Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 – 03:39 PM EDT

PDB ID	:	4OU2
Title	:	A 2.15 Angstroms X-ray crystal structure of E268A 2-aminomuconate 6-semialdehyde dehydrogenase catalytic intermediate from Pseudomonas fluorescens
Authors	:	Huo, L.; Liu, A.
Deposited on	:	2014-02-14
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

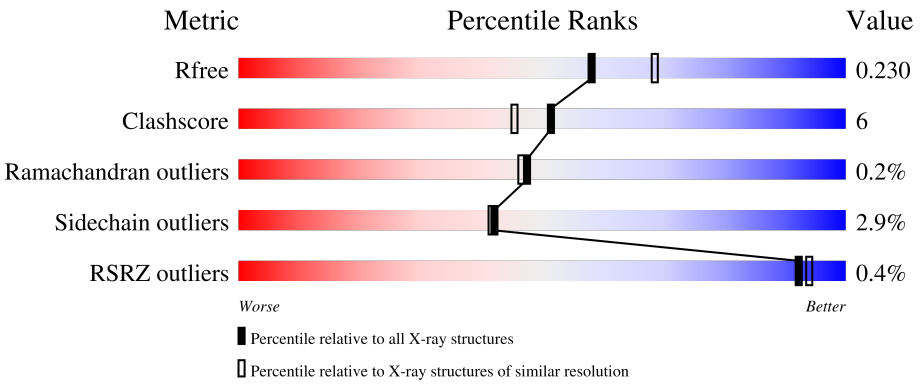
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	483	92% 8%
1	B	483	87% 11% •
1	C	483	% 84% 14% •
1	D	483	89% 11% •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	6OA	B	603	-	-	X	-
4	6OA	C	603	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16024 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.

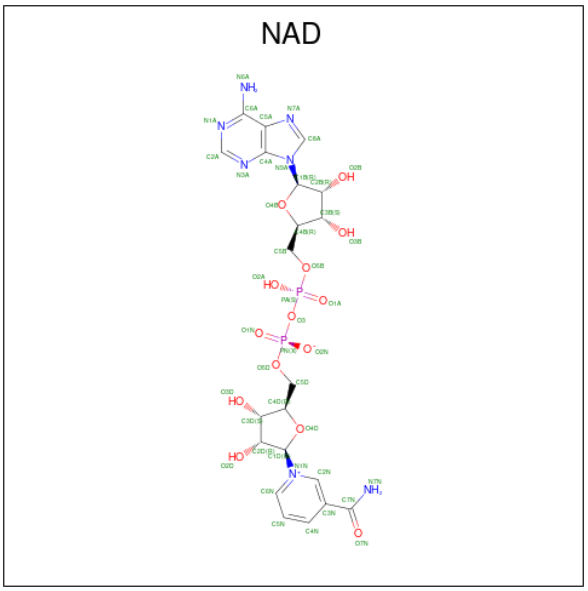
- Molecule 1 is a protein called 2-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	3667	2319	637	699	12	0	0	0
1	B	483	3667	2319	637	699	12	0	0	0
1	C	483	3667	2319	637	699	12	0	0	0
1	D	483	3667	2319	637	699	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	GLU	engineered mutation	UNP Q83V33
B	268	ALA	GLU	engineered mutation	UNP Q83V33
C	268	ALA	GLU	engineered mutation	UNP Q83V33
D	268	ALA	GLU	engineered mutation	UNP Q83V33

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

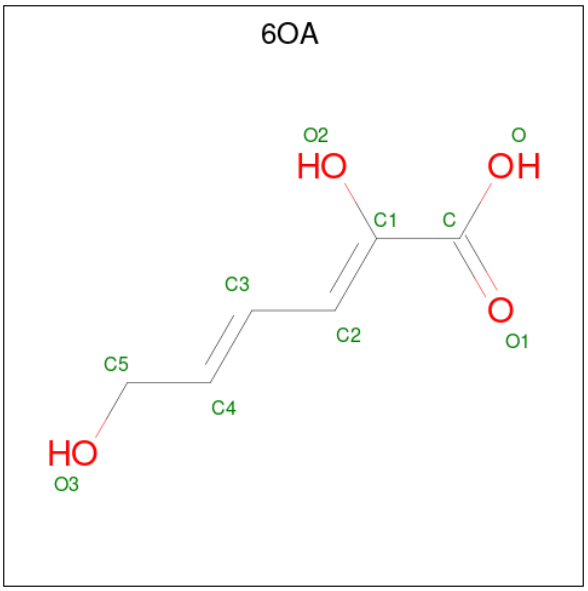


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is (2Z,4E)-2,6-dihydroxyhexa-2,4-dienoic acid (three-letter code: 6OA) (formula: $C_6H_8O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	B	1	10	6	4	0	0
			Total	C	O		
4	C	1	10	6	4	0	0
			Total	C	O		
4	D	1	10	6	4	0	0

- Molecule 5 is water.

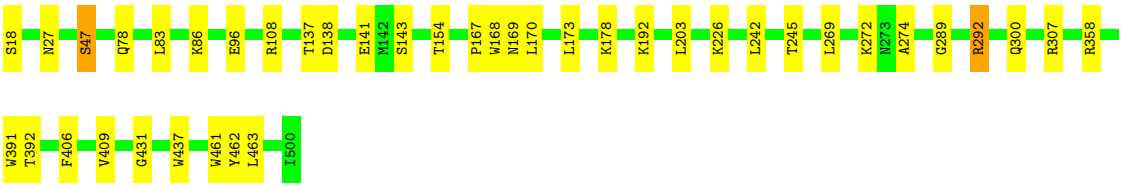
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	342	342	342	0	0
			Total	O		
5	B	308	308	308	0	0
			Total	O		
5	C	207	207	207	0	0
			Total	O		
5	D	279	279	279	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

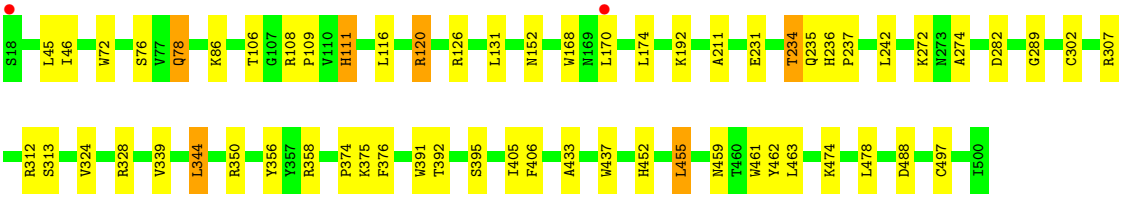
• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain A:



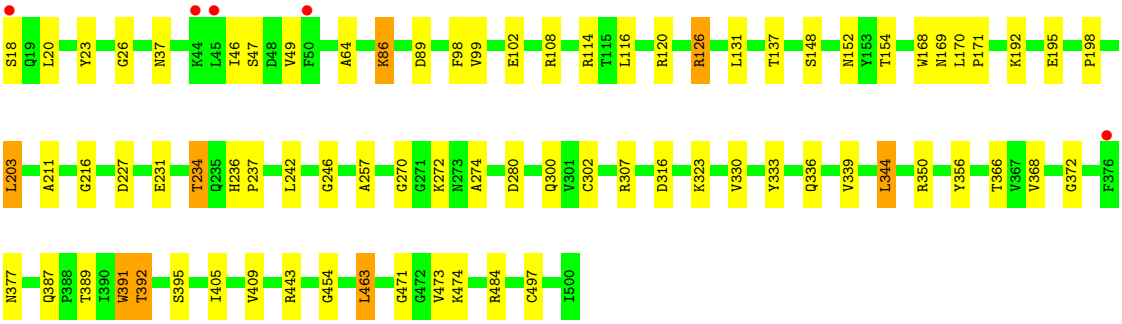
• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain B:



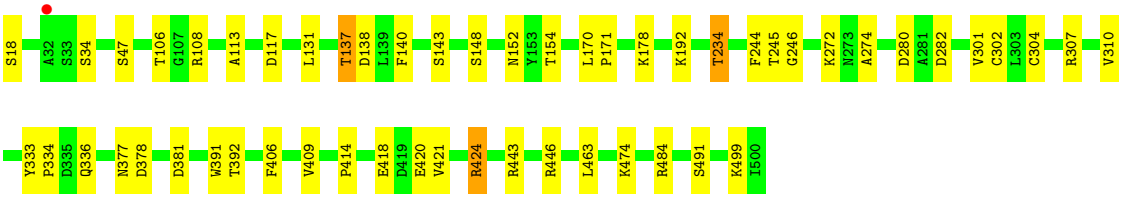
• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain C:



• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain D:


S18
A32
S33
S34
S47
T106
G107
R108
A113
D117
L131
T137
D138
L139
F140
S143
S148
N152
Y153
T154
L170
P171
K178
K192
T234
F244
T245
G246
K272
N273
A274
D280
A281
D282
V301
C302
L303
C304
R307
V310
Y333
P334
D335
Q336
N377
D378
D381
W391
T392
F406
V409
P414
E418
D419
E420
V421
R424
R443
R446
L463
K474
R484
S491
K499
I500

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.57Å 141.56Å 174.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.93 – 2.15 42.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.93-2.15) 91.1 (42.93-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.192 , 0.235 0.182 , 0.230	Depositor DCC
R_{free} test set	6008 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16024	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 6OA, NA

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	0.94	3/3746 (0.1%)	0.79	2/5093 (0.0%)
1	B	0.97	6/3746 (0.2%)	0.80	2/5093 (0.0%)
1	C	0.87	2/3746 (0.1%)	0.76	0/5093
1	D	0.87	0/3746	0.77	1/5093 (0.0%)
All	All	0.91	11/14984 (0.1%)	0.78	5/20372 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	391	TRP	CD2-CE2	5.97	1.48	1.41
1	B	462	TYR	CZ-OH	5.83	1.47	1.37
1	B	462	TYR	CE2-CZ	5.58	1.45	1.38
1	B	391	TRP	CD2-CE2	5.57	1.48	1.41
1	A	461	TRP	CD2-CE2	5.45	1.47	1.41
1	B	461	TRP	CD2-CE2	5.44	1.47	1.41
1	A	462	TYR	CE2-CZ	5.37	1.45	1.38
1	B	72	TRP	CD2-CE2	5.37	1.47	1.41
1	C	168	TRP	CD2-CE2	5.31	1.47	1.41
1	B	168	TRP	CD2-CE2	5.18	1.47	1.41
1	A	168	TRP	CD2-CE2	5.13	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	46	ILE	CB-CA-C	-5.94	99.73	111.60
1	A	292	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	173	LEU	CB-CG-CD2	5.33	120.06	111.00
1	D	282	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	462	TYR	OH-CZ-CE2	5.06	133.76	120.10

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	3667	0	3603	22	0
1	B	3667	0	3603	43	0
1	C	3667	0	3603	54	0
1	D	3667	0	3603	33	0
2	A	44	0	26	6	0
2	B	44	0	26	8	0
2	C	44	0	26	14	0
2	D	44	0	26	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	5	3	0
4	B	10	0	4	4	0
4	C	10	0	4	4	0
4	D	10	0	4	2	0
5	A	342	0	0	8	0
5	B	308	0	0	5	0
5	C	207	0	0	4	0
5	D	279	0	0	4	0
All	All	16024	0	14533	165	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 (165) 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)
2:B:601:NAD:C4N	4:B:603:6OA:C5	2.39	1.00
2:A:601:NAD:C4N	4:A:603:6OA:H6	1.95	0.96
2:C:601:NAD:C4N	4:C:603:6OA:C5	2.45	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:NAD:H4N	4:A:603:6OA:H6	1.55	0.87
2:C:601:NAD:H4N	4:C:603:6OA:C5	2.05	0.86
1:B:234:THR:HG21	5:B:832:HOH:O	1.77	0.84
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.60	0.83
1:C:169:ASN:HD21	2:C:601:NAD:H5N	1.42	0.82
1:B:111:HIS:HD2	5:B:765:HOH:O	1.62	0.82
1:D:280:ASP:OD2	1:D:443:ARG:NH1	2.15	0.78
1:B:111:HIS:H	1:B:111:HIS:CD2	2.02	0.77
2:C:601:NAD:C4N	4:C:603:6OA:O3	2.32	0.76
2:B:601:NAD:H4N	4:B:603:6OA:C5	2.15	0.75
1:C:389:THR:HB	1:C:409:VAL:HG23	1.67	0.75
1:C:366:THR:HB	1:C:392:THR:HG22	1.70	0.74
1:B:358:ARG:NH2	5:B:791:HOH:O	2.09	0.74
1:B:111:HIS:CD2	5:B:765:HOH:O	2.41	0.71
1:A:96:GLU:OE2	5:A:939:HOH:O	2.08	0.70
1:A:27:ASN:ND2	5:A:979:HOH:O	2.22	0.70
1:C:169:ASN:ND2	2:C:601:NAD:H5N	2.07	0.70
1:D:491:SER:O	5:D:705:HOH:O	2.09	0.70
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.74	0.69
1:D:421:VAL:HA	1:D:424:ARG:HG3	1.75	0.69
1:D:420:GLU:O	1:D:424:ARG:HG2	1.92	0.69
1:C:280:ASP:OD2	1:C:443:ARG:NH1	2.27	0.68
1:A:141:GLU:OE1	5:A:956:HOH:O	2.11	0.66
1:C:377:ASN:OD1	5:C:873:HOH:O	2.13	0.66
2:D:601:NAD:C4N	4:D:603:6OA:C5	2.73	0.65
1:C:272:LYS:HG3	1:C:307:ARG:CD	2.27	0.65
1:A:18:SER:HB3	1:A:47:SER:HB3	1.80	0.64
1:D:418:GLU:OE2	1:D:446:ARG:HD2	1.97	0.64
2:A:601:NAD:O1N	5:A:959:HOH:O	2.15	0.64
2:B:601:NAD:C5N	4:B:603:6OA:O3	2.45	0.64
1:B:86:LYS:NZ	1:B:211:ALA:O	2.31	0.64
2:C:601:NAD:C5N	4:C:603:6OA:O3	2.47	0.62
1:D:18:SER:HB3	1:D:47:SER:HB3	1.81	0.62
1:C:333:TYR:HB2	1:C:336:GLN:HB2	1.82	0.61
1:D:418:GLU:OE1	1:D:446:ARG:NH1	2.34	0.60
1:A:292:ARG:NH1	5:A:951:HOH:O	2.33	0.60
1:D:474:LYS:O	5:D:704:HOH:O	2.17	0.60
1:B:111:HIS:HD2	1:B:111:HIS:H	1.50	0.59
1:D:420:GLU:O	1:D:424:ARG:CG	2.50	0.59
1:B:109:PRO:HB3	1:B:111:HIS:NE2	2.18	0.59
1:B:478:LEU:HD23	1:B:478:LEU:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:LYS:HE2	1:D:245:THR:OG1	2.04	0.58
1:B:106:THR:OG1	1:B:108:ARG:HD2	2.04	0.57
2:D:601:NAD:H4N	4:D:603:6OA:C5	2.34	0.57
1:B:406:PHE:CE2	2:B:601:NAD:H2D	2.40	0.56
1:C:272:LYS:CG	1:C:307:ARG:HD2	2.35	0.56
1:A:269:LEU:O	2:A:601:NAD:H2N	2.06	0.56
1:B:344:LEU:HD23	1:B:350:ARG:HA	1.88	0.56
1:C:344:LEU:HD23	1:C:350:ARG:HA	1.88	0.56
1:D:234:THR:HG21	5:D:850:HOH:O	2.06	0.55
1:A:27:ASN:HB2	5:A:979:HOH:O	2.07	0.55
1:C:20:LEU:HD12	1:C:49:VAL:HG22	1.89	0.54
1:C:108:ARG:NH2	1:C:170:LEU:HD23	2.23	0.54
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.89	0.53
1:C:102:GLU:OE2	1:C:171:PRO:HB2	2.07	0.53
1:B:78:GLN:H	1:B:78:GLN:CD	2.10	0.52
1:C:316:ASP:N	5:C:901:HOH:O	2.42	0.52
1:C:86:LYS:HD3	5:C:819:HOH:O	2.08	0.52
1:C:302:CYS:SG	2:C:601:NAD:C7N	2.97	0.52
1:A:108:ARG:NH2	1:A:170:LEU:HD23	2.25	0.52
1:C:302:CYS:SG	2:C:601:NAD:C3N	2.98	0.52
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.91	0.52
1:C:86:LYS:NZ	1:C:211:ALA:O	2.42	0.52
1:B:452:HIS:ND1	1:B:474:LYS:HE2	2.26	0.51
1:B:111:HIS:CE1	1:B:339:VAL:O	2.63	0.50
1:B:302:CYS:HB3	2:B:601:NAD:C6N	2.41	0.50
1:C:169:ASN:HB2	1:C:300:GLN:O	2.11	0.50
1:A:391:TRP:CH2	1:A:409:VAL:HG21	2.46	0.50
1:C:302:CYS:SG	2:C:601:NAD:C4N	2.98	0.50
1:C:323:LYS:HE2	1:C:368:VAL:O	2.11	0.50
1:D:302:CYS:SG	2:D:601:NAD:C7N	2.99	0.50
2:A:601:NAD:C4N	4:A:603:6OA:C5	2.81	0.50
1:B:111:HIS:CD2	1:B:111:HIS:N	2.78	0.50
1:B:111:HIS:NE2	1:B:339:VAL:HG13	2.27	0.49
1:D:406:PHE:CE2	2:D:601:NAD:H2D	2.46	0.49
1:B:282:ASP:OD1	1:B:282:ASP:C	2.50	0.49
1:C:484:ARG:NH1	1:D:484:ARG:NH1	2.61	0.49
1:C:302:CYS:HB3	2:C:601:NAD:C2N	2.42	0.49
1:C:137:THR:HB	1:C:154:THR:OG1	2.14	0.48
1:C:356:TYR:CG	1:C:405:ILE:HG12	2.49	0.48
1:B:116:LEU:O	1:B:120:ARG:HB2	2.12	0.48
2:B:601:NAD:C4N	4:B:603:6OA:O3	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HG3	1:A:307:ARG:CD	2.42	0.48
1:C:89:ASP:OD1	1:C:126:ARG:NH2	2.37	0.48
1:C:98:PHE:CE1	1:C:203:LEU:HB3	2.49	0.47
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.48	0.47
1:A:358:ARG:HD3	5:A:878:HOH:O	2.13	0.47
1:C:64:ALA:HA	1:C:216:GLY:O	2.15	0.47
1:B:356:TYR:CG	1:B:405:ILE:HG12	2.50	0.47
1:C:231:GLU:O	1:C:234:THR:HG22	2.15	0.47
1:D:143:SER:OG	5:D:954:HOH:O	2.21	0.47
1:A:83:LEU:O	1:A:86:LYS:HB3	2.14	0.46
1:B:274:ALA:HA	1:B:307:ARG:O	2.15	0.46
1:B:108:ARG:NH2	1:B:170:LEU:HD23	2.31	0.46
1:C:372:GLY:O	1:C:387:GLN:HG3	2.16	0.46
1:D:137:THR:HB	1:D:138:ASP:H	1.64	0.46
1:C:302:CYS:HB3	2:C:601:NAD:C3N	2.45	0.46
1:B:302:CYS:CB	2:B:601:NAD:C3N	2.94	0.46
1:D:113:ALA:HA	1:D:117:ASP:HB2	1.98	0.46
1:B:272:LYS:O	1:B:307:ARG:HD3	2.15	0.45
1:C:169:ASN:HD21	2:C:601:NAD:C5N	2.20	0.45
1:D:333:TYR:HB2	1:D:336:GLN:HB2	1.99	0.45
1:D:137:THR:HB	1:D:154:THR:OG1	2.16	0.45
1:B:120:ARG:HA	1:B:120:ARG:HD2	1.76	0.45
1:C:102:GLU:OE1	1:C:171:PRO:HD2	2.16	0.45
1:C:18:SER:HB3	1:C:47:SER:HB3	1.98	0.45
1:C:246:GLY:HA2	2:C:601:NAD:O4D	2.16	0.45
1:B:106:THR:CB	1:B:108:ARG:HH11	2.29	0.45
1:A:289:GLY:HA3	1:A:437:TRP:CZ2	2.53	0.44
1:C:23:TYR:CZ	1:C:26:GLY:HA2	2.52	0.44
1:B:231:GLU:O	1:B:234:THR:HG22	2.18	0.44
1:D:140:PHE:HB2	1:D:152:ASN:HB2	2.00	0.44
1:C:473:VAL:HG23	1:C:474:LYS:HG3	2.00	0.44
1:A:178:LYS:HE2	1:A:245:THR:OG1	2.18	0.43
1:C:152:ASN:OD1	1:C:497:CYS:HB2	2.19	0.43
1:B:289:GLY:HA3	1:B:437:TRP:CZ2	2.54	0.43
1:C:454:GLY:HA3	1:C:471:GLY:O	2.19	0.43
1:D:108:ARG:NH2	1:D:170:LEU:HD23	2.33	0.43
1:D:301:VAL:HB	1:D:304:CYS:SG	2.59	0.43
1:C:99:VAL:HG21	1:C:114:ARG:HG2	2.01	0.43
1:A:292:ARG:CZ	5:A:951:HOH:O	2.67	0.43
1:C:391:TRP:CH2	1:C:409:VAL:HG21	2.54	0.43
1:C:274:ALA:HA	1:C:307:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HH22	1:A:170:LEU:HD23	1.84	0.42
1:D:244:PHE:CZ	1:D:246:GLY:HA3	2.54	0.42
1:C:474:LYS:HB3	5:C:774:HOH:O	2.19	0.42
1:B:234:THR:HG22	1:B:235:GLN:HG3	2.00	0.42
1:C:116:LEU:O	1:C:120:ARG:HB2	2.19	0.42
1:C:236:HIS:HA	1:C:237:PRO:HD3	1.81	0.42
1:B:152:ASN:OD1	1:B:497:CYS:HB2	2.19	0.42
1:D:148:SER:HB2	1:D:499:LYS:NZ	2.34	0.42
1:B:324:VAL:O	1:B:328:ARG:HG3	2.19	0.42
1:C:330:VAL:HB	1:C:339:VAL:HA	2.01	0.42
1:D:148:SER:HB2	1:D:499:LYS:HZ1	1.85	0.42
1:A:137:THR:HB	1:A:154:THR:OG1	2.20	0.42
1:D:378:ASP:OD1	1:D:378:ASP:C	2.58	0.42
1:B:236:HIS:HA	1:B:237:PRO:HD3	1.83	0.41
1:D:108:ARG:HH22	1:D:170:LEU:HD23	1.85	0.41
1:A:274:ALA:HA	1:A:307:ARG:O	2.20	0.41
1:B:312:ARG:HG3	1:B:313:SER:N	2.35	0.41
1:B:488:ASP:O	5:B:703:HOH:O	2.21	0.41
1:B:374:PRO:HG2	1:B:376:PHE:CE2	2.55	0.41
1:C:108:ARG:HH22	1:C:170:LEU:HD23	1.86	0.41
1:C:234:THR:HG23	1:C:257:ALA:HB1	2.02	0.41
1:A:406:PHE:CE2	2:A:601:NAD:H2D	2.56	0.41
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.84	0.41
1:B:302:CYS:SG	2:B:601:NAD:C3N	3.09	0.41
1:C:270:GLY:HA2	2:C:601:NAD:O2D	2.21	0.41
1:D:274:ALA:HA	1:D:307:ARG:O	2.21	0.41
1:B:76:SER:OG	1:B:78:GLN:HG2	2.20	0.41
1:B:433:ALA:HA	1:B:455:LEU:O	2.21	0.41
1:C:20:LEU:CD1	1:C:198:PRO:HG2	2.51	0.41
1:C:463:LEU:HD23	1:C:463:LEU:HA	1.96	0.41
1:D:377:ASN:N	1:D:381:ASP:OD2	2.54	0.41
1:A:169:ASN:HB2	1:A:300:GLN:O	2.21	0.40
1:B:272:LYS:HG3	1:B:307:ARG:CD	2.50	0.40
1:C:37:ASN:ND2	1:C:46:ILE:HD12	2.36	0.40
1:B:437:TRP:CE3	1:B:459:ASN:HA	2.57	0.40
1:D:310:VAL:O	1:D:414:PRO:HA	2.22	0.40
1:A:137:THR:HB	1:A:138:ASP:H	1.77	0.40
1:C:195:GLU:OE1	1:C:195:GLU:N	2.41	0.40
1:D:106:THR:OG1	1:D:108:ARG:HD2	2.21	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	481/483 (100%)	459 (95%)	20 (4%)	2 (0%)	34	29
1	B	481/483 (100%)	460 (96%)	21 (4%)	0	100	100
1	C	481/483 (100%)	460 (96%)	21 (4%)	0	100	100
1	D	481/483 (100%)	463 (96%)	17 (4%)	1 (0%)	47	46
All	All	1924/1932 (100%)	1842 (96%)	79 (4%)	3 (0%)	47	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	A	431	GLY
1	D	171	PRO

5.3.2 Protein sidechains (i)

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	391/391 (100%)	382 (98%)	9 (2%)	50	53
1	B	391/391 (100%)	376 (96%)	15 (4%)	33	31
1	C	391/391 (100%)	378 (97%)	13 (3%)	38	37
1	D	391/391 (100%)	382 (98%)	9 (2%)	50	53
All	All	1564/1564 (100%)	1518 (97%)	46 (3%)	42	42

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	78	GLN
1	A	143	SER
1	A	192	LYS
1	A	203	LEU
1	A	226	LYS
1	A	242	LEU
1	A	392	THR
1	A	463	LEU
1	B	45	LEU
1	B	78	GLN
1	B	111	HIS
1	B	120	ARG
1	B	126	ARG
1	B	131	LEU
1	B	192	LYS
1	B	234	THR
1	B	242	LEU
1	B	344	LEU
1	B	375	LYS
1	B	392	THR
1	B	395	SER
1	B	455	LEU
1	B	463	LEU
1	C	86	LYS
1	C	126	ARG
1	C	131	LEU
1	C	148	SER
1	C	192	LYS
1	C	203	LEU
1	C	227	ASP
1	C	234	THR
1	C	242	LEU
1	C	344	LEU
1	C	392	THR
1	C	395	SER
1	C	463	LEU
1	D	34	SER
1	D	131	LEU
1	D	137	THR
1	D	192	LYS
1	D	234	THR
1	D	334	PRO

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Mol	Chain	Res	Type
1	D	392	THR
1	D	424	ARG
1	D	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
4	6OA	C	603	1	9,9,9	2.01	3 (33%)	8,10,10	3.38	4 (50%)
4	6OA	A	603	1	9,9,9	1.54	2 (22%)	8,10,10	3.89	4 (50%)
2	NAD	B	601	-	42,48,48	1.78	9 (21%)	50,73,73	2.01	13 (26%)
2	NAD	D	601	-	42,48,48	1.51	6 (14%)	50,73,73	1.34	6 (12%)
2	NAD	A	601	-	42,48,48	1.75	9 (21%)	50,73,73	1.86	11 (22%)
4	6OA	B	603	1	9,9,9	2.51	4 (44%)	8,10,10	3.83	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	C	601	-	42,48,48	1.29	4 (9%)	50,73,73	1.41	5 (10%)
4	6OA	D	603	1	9,9,9	3.00	3 (33%)	8,10,10	4.17	4 (50%)

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
4	6OA	C	603	1	-	0/8/9/9	-
4	6OA	A	603	1	-	0/8/9/9	-
2	NAD	B	601	-	-	8/26/62/62	0/5/5/5
2	NAD	D	601	-	-	6/26/62/62	0/5/5/5
2	NAD	A	601	-	-	5/26/62/62	0/5/5/5
4	6OA	B	603	1	-	0/8/9/9	-
2	NAD	C	601	-	-	5/26/62/62	0/5/5/5
4	6OA	D	603	1	-	0/8/9/9	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	6OA	C1-C	-6.62	1.40	1.48
2	D	601	NAD	C7N-N7N	5.64	1.43	1.33
2	A	601	NAD	C7N-N7N	5.29	1.43	1.33
2	B	601	NAD	C7N-N7N	5.27	1.43	1.33
4	D	603	6OA	O1-C	4.85	1.35	1.22
4	B	603	6OA	O1-C	4.84	1.35	1.22
4	C	603	6OA	C5-C4	-4.45	1.40	1.49
2	B	601	NAD	C2B-C1B	-3.61	1.48	1.53
4	B	603	6OA	C2-C1	-3.57	1.31	1.39
2	A	601	NAD	C2A-N3A	3.55	1.37	1.32
2	A	601	NAD	C2D-C1D	-3.30	1.48	1.53
2	B	601	NAD	C2D-C1D	-3.25	1.48	1.53
4	D	603	6OA	O-C	-3.22	1.21	1.30
4	A	603	6OA	C2-C1	-3.22	1.32	1.39
4	B	603	6OA	C1-C	-3.21	1.44	1.48
2	B	601	NAD	C6N-N1N	3.14	1.43	1.35
4	B	603	6OA	O-C	-3.09	1.21	1.30
2	A	601	NAD	C6A-N6A	3.07	1.45	1.34
2	B	601	NAD	C6A-N6A	3.01	1.45	1.34
2	B	601	NAD	C2A-N3A	2.94	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	C2N-N1N	-2.90	1.31	1.35
2	C	601	NAD	C2D-C1D	-2.88	1.49	1.53
2	A	601	NAD	C3N-C7N	2.85	1.54	1.50
2	D	601	NAD	C2D-C1D	-2.75	1.49	1.53
2	D	601	NAD	C2A-N3A	2.70	1.36	1.32
2	A	601	NAD	O7N-C7N	2.53	1.29	1.24
2	D	601	NAD	C6A-N6A	2.53	1.43	1.34
2	C	601	NAD	C4A-N3A	-2.48	1.32	1.35
2	A	601	NAD	C2N-N1N	2.39	1.37	1.35
4	C	603	6OA	C1-C	-2.35	1.45	1.48
2	A	601	NAD	PA-O1A	2.34	1.59	1.50
2	B	601	NAD	O4B-C4B	-2.32	1.39	1.45
2	B	601	NAD	O3D-C3D	-2.25	1.37	1.43
2	A	601	NAD	O3B-C3B	-2.22	1.37	1.43
2	B	601	NAD	C2N-N1N	2.17	1.37	1.35
2	C	601	NAD	PA-O2A	-2.12	1.45	1.55
4	C	603	6OA	C2-C1	-2.10	1.35	1.39
2	D	601	NAD	PA-O1A	2.09	1.58	1.50
2	D	601	NAD	O4B-C1B	2.08	1.44	1.41
4	A	603	6OA	C3-C2	2.01	1.49	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	6OA	O2-C1-C	9.23	119.60	114.01
4	D	603	6OA	O-C-C1	8.44	124.06	115.91
4	B	603	6OA	O-C-C1	7.96	123.60	115.91
4	D	603	6OA	O2-C1-C	6.90	118.19	114.01
4	C	603	6OA	O2-C1-C	6.57	117.99	114.01
2	A	601	NAD	O2A-PA-O1A	-6.34	80.90	112.24
4	B	603	6OA	O2-C1-C	6.28	117.81	114.01
2	B	601	NAD	N3A-C2A-N1A	-5.92	119.43	128.68
2	B	601	NAD	C3N-C2N-N1N	-5.62	114.93	120.43
4	C	603	6OA	O3-C5-C4	4.84	125.63	112.06
2	D	601	NAD	N3A-C2A-N1A	-4.53	121.59	128.68
2	A	601	NAD	O5B-PA-O1A	-4.51	91.45	109.07
2	A	601	NAD	N3A-C2A-N1A	-4.48	121.67	128.68
2	B	601	NAD	C2N-C3N-C4N	4.28	123.11	118.26
2	C	601	NAD	C4A-C5A-N7A	-4.21	105.01	109.40
2	B	601	NAD	PN-O3-PA	-4.12	118.68	132.83
2	C	601	NAD	O4B-C1B-C2B	-4.02	101.06	106.93
2	A	601	NAD	PN-O3-PA	-3.92	119.39	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NAD	O4D-C1D-C2D	-3.86	101.29	106.93
2	D	601	NAD	C3N-C2N-N1N	-3.81	116.70	120.43
2	C	601	NAD	C3N-C7N-N7N	-3.81	113.18	117.75
4	C	603	6OA	O-C-C1	3.71	119.49	115.91
4	A	603	6OA	O-C-C1	3.59	119.38	115.91
2	A	601	NAD	O4D-C1D-C2D	-3.44	101.89	106.93
2	B	601	NAD	C5N-C6N-N1N	3.33	125.18	120.40
2	B	601	NAD	C3N-C7N-N7N	-3.30	113.79	117.75
2	A	601	NAD	C5N-C4N-C3N	3.21	124.15	120.34
2	B	601	NAD	O7N-C7N-C3N	3.15	123.40	119.63
2	B	601	NAD	C6N-N1N-C2N	-3.03	119.21	121.97
4	A	603	6OA	C2-C3-C4	-2.95	116.72	123.63
4	D	603	6OA	O-C-O1	-2.94	116.88	123.61
2	B	601	NAD	C6N-C5N-C4N	-2.92	115.20	119.44
2	A	601	NAD	O7N-C7N-C3N	2.83	123.02	119.63
2	D	601	NAD	PN-O3-PA	-2.83	123.13	132.83
2	D	601	NAD	C4A-C5A-N7A	-2.82	106.46	109.40
2	D	601	NAD	O2D-C2D-C3D	2.68	120.50	111.82
2	A	601	NAD	O7N-C7N-N7N	-2.65	118.81	122.58
2	D	601	NAD	O7N-C7N-C3N	2.62	122.76	119.63
4	B	603	6OA	O-C-O1	-2.61	117.64	123.61
2	B	601	NAD	C2A-N1A-C6A	2.55	123.11	118.75
4	D	603	6OA	C2-C3-C4	-2.52	117.73	123.63
2	B	601	NAD	O5D-PN-O1N	-2.42	99.60	109.07
2	C	601	NAD	N3A-C2A-N1A	-2.26	125.15	128.68
2	A	601	NAD	C6N-C5N-C4N	-2.26	116.16	119.44
4	B	603	6OA	O2-C1-C2	-2.24	119.02	122.92
2	B	601	NAD	O5D-C5D-C4D	-2.22	101.35	108.99
4	A	603	6OA	O-C-O1	-2.18	118.61	123.61
2	A	601	NAD	O2D-C2D-C3D	2.16	118.80	111.82
4	C	603	6OA	O-C-O1	-2.07	118.88	123.61
2	B	601	NAD	O2D-C2D-C3D	2.03	118.38	111.82
2	A	601	NAD	C2D-C3D-C4D	-2.00	98.75	102.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C5B-O5B-PA-O3
2	B	601	NAD	C5B-O5B-PA-O2A
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	C	601	NAD	C5B-O5B-PA-O1A
2	C	601	NAD	C5B-O5B-PA-O3
2	D	601	NAD	C5B-O5B-PA-O3
2	A	601	NAD	O4B-C4B-C5B-O5B
2	A	601	NAD	C3B-C4B-C5B-O5B
2	C	601	NAD	C3D-C4D-C5D-O5D
2	D	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	PA-O3-PN-O5D
2	A	601	NAD	C4D-C5D-O5D-PN
2	B	601	NAD	C5B-O5B-PA-O3
2	A	601	NAD	C5B-O5B-PA-O1A
2	B	601	NAD	C5B-O5B-PA-O1A
2	C	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C3D-C4D-C5D-O5D
2	D	601	NAD	C5B-O5B-PA-O1A
2	D	601	NAD	C5B-O5B-PA-O2A
2	C	601	NAD	O4D-C4D-C5D-O5D

There are no ring outliers.

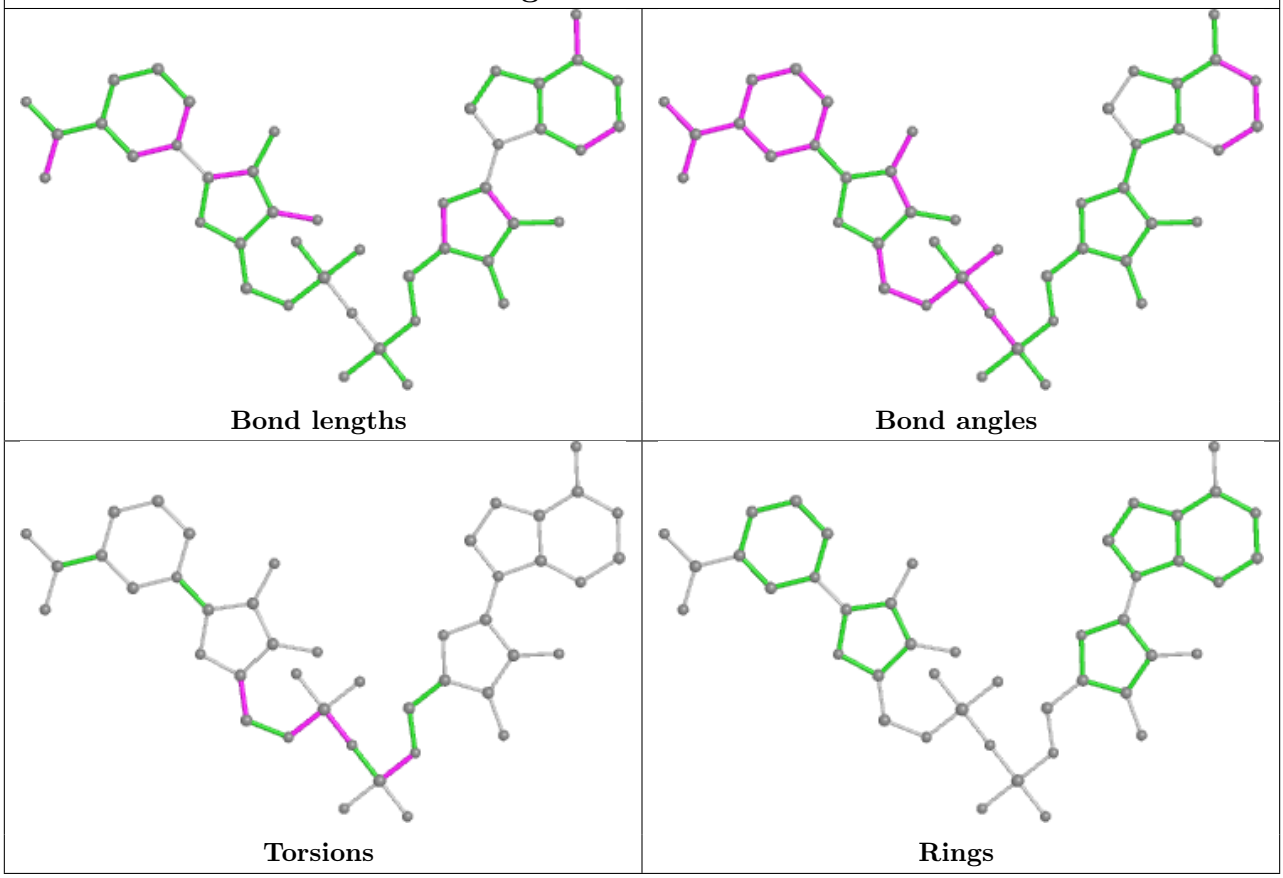
8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	6OA	4	0
4	A	603	6OA	3	0
2	B	601	NAD	8	0
2	D	601	NAD	4	0
2	A	601	NAD	6	0
4	B	603	6OA	4	0
2	C	601	NAD	14	0
4	D	603	6OA	2	0

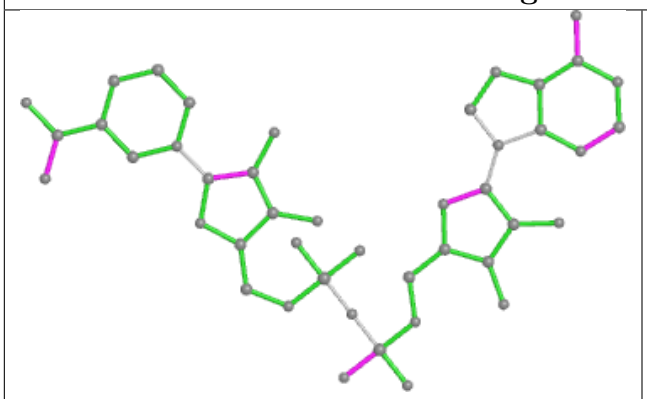
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

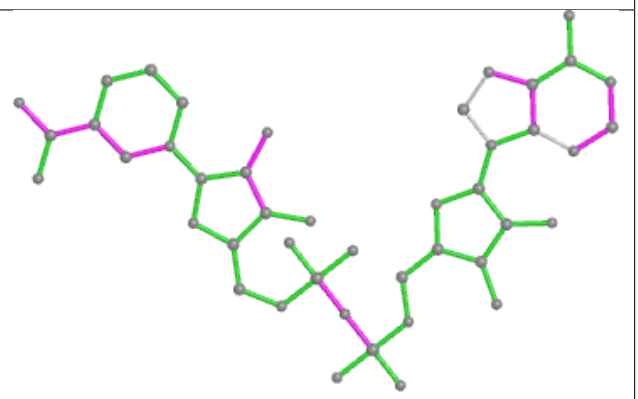
Ligand NAD B 601



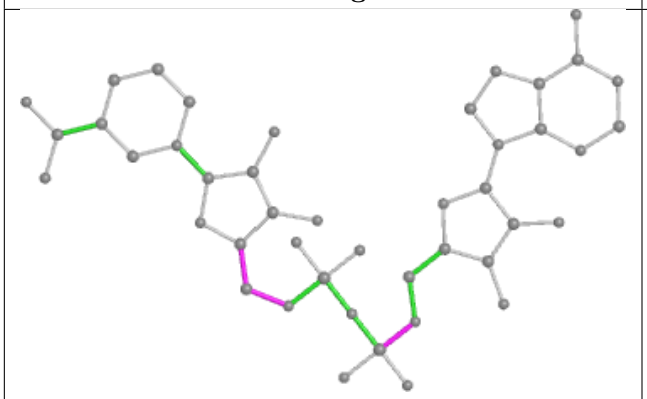
Ligand NAD D 601



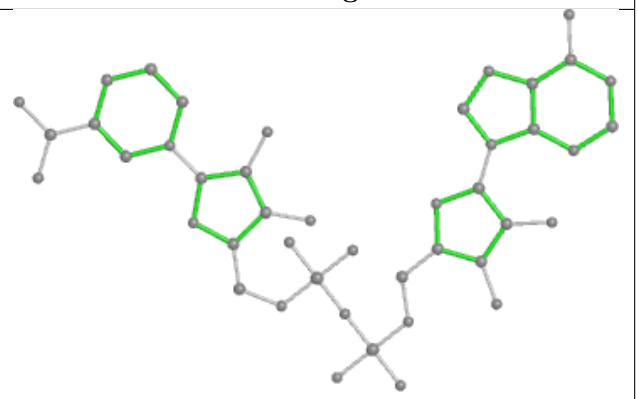
Bond lengths



Bond angles

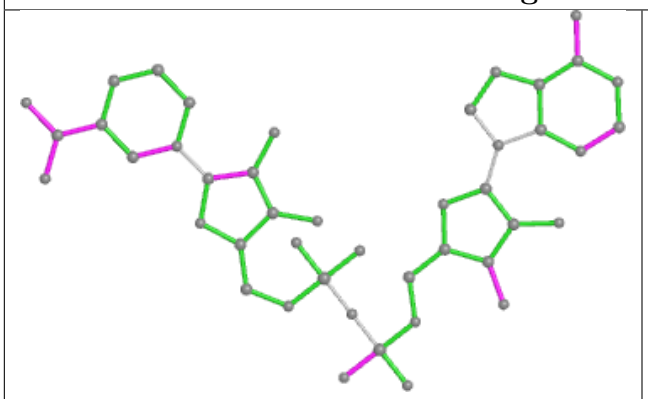


Torsions

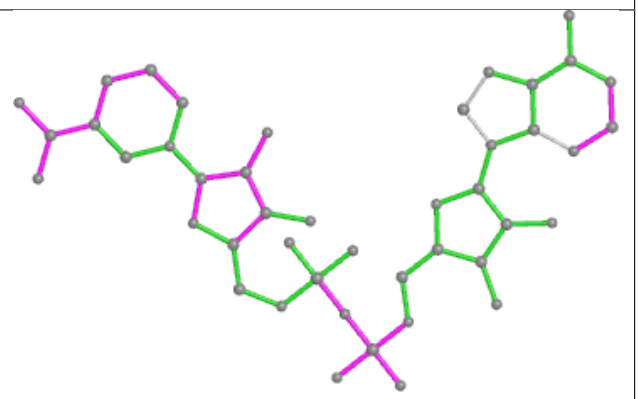


Rings

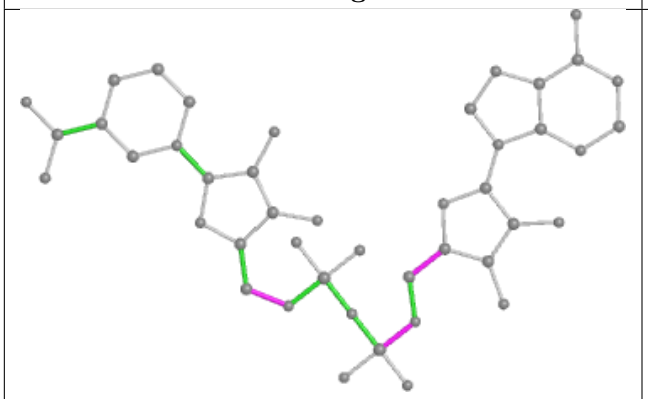
Ligand NAD A 601



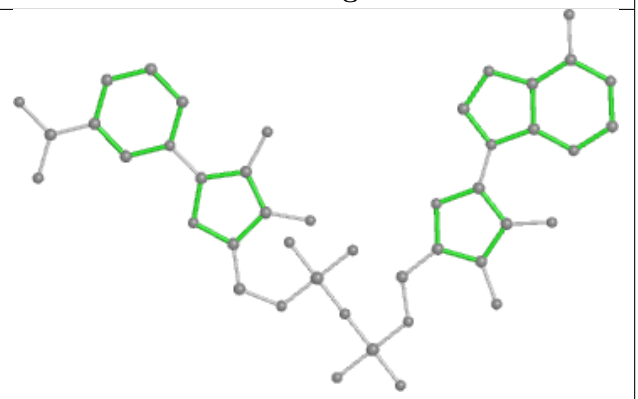
Bond lengths



Bond angles

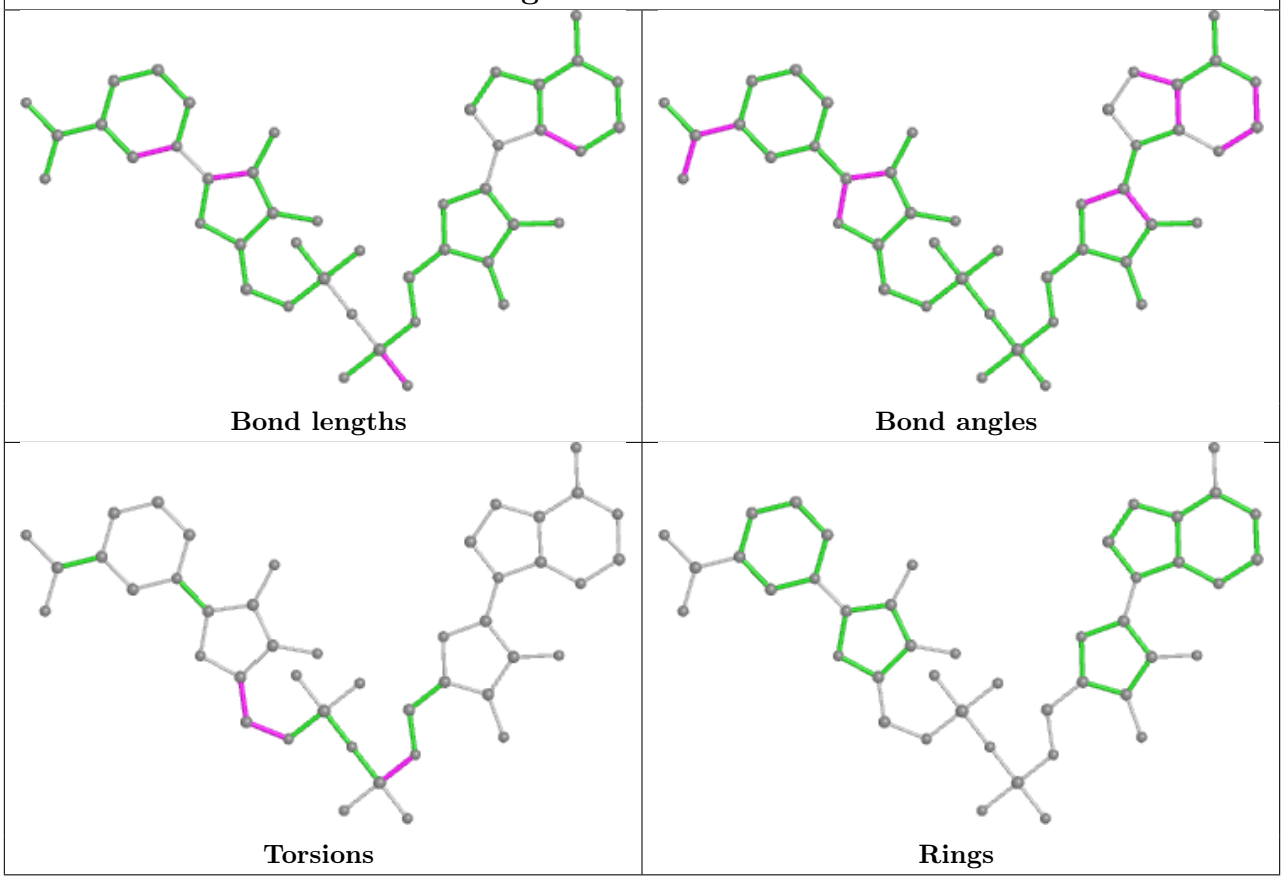


Torsions



Rings

Ligand NAD C 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	483/483 (100%)	-0.42	0	100	100	17, 25, 35, 47	0
1	B	483/483 (100%)	-0.37	2 (0%)	92	94	16, 25, 36, 52	0
1	C	483/483 (100%)	-0.20	5 (1%)	82	86	19, 34, 48, 65	0
1	D	483/483 (100%)	-0.41	1 (0%)	95	96	18, 28, 39, 50	0
All	All	1932/1932 (100%)	-0.35	8 (0%)	92	94	16, 28, 43, 65	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	SER	5.8
1	C	18	SER	3.5
1	C	44	LYS	3.1
1	C	45	LEU	2.8
1	C	376	PHE	2.7
1	B	170	LEU	2.1
1	C	50	PHE	2.1
1	D	32	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

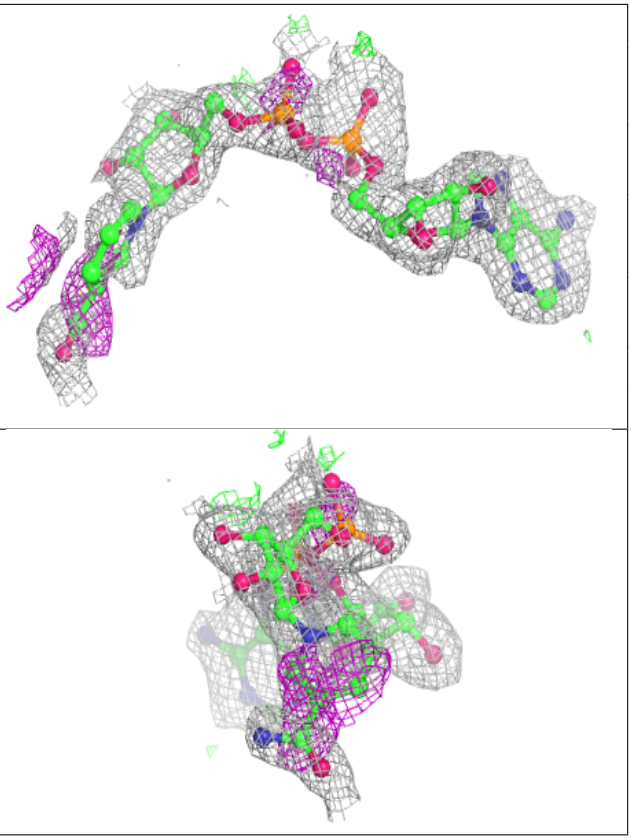
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

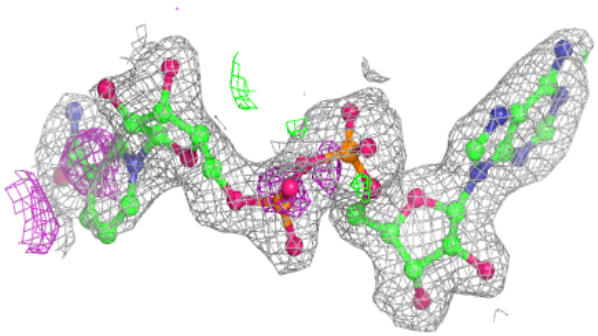
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	C	602	1/1	0.77	0.21	49,49,49,49	0
3	NA	B	602	1/1	0.84	0.18	41,41,41,41	0
3	NA	D	602	1/1	0.85	0.24	49,49,49,49	0
4	6OA	C	603	10/10	0.90	0.14	24,26,27,28	0
2	NAD	C	601	44/44	0.91	0.13	33,48,56,72	0
4	6OA	D	603	10/10	0.92	0.12	22,24,25,25	0
2	NAD	D	601	44/44	0.93	0.14	30,43,50,56	0
2	NAD	B	601	44/44	0.93	0.12	24,37,54,62	0
4	6OA	A	603	10/10	0.94	0.11	22,24,26,27	0
4	6OA	B	603	10/10	0.94	0.12	23,24,26,26	0
2	NAD	A	601	44/44	0.95	0.10	24,36,44,47	0
3	NA	A	602	1/1	0.96	0.16	33,33,33,33	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 601:

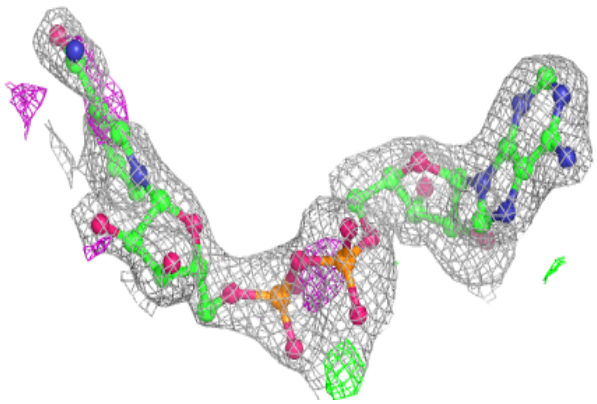
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

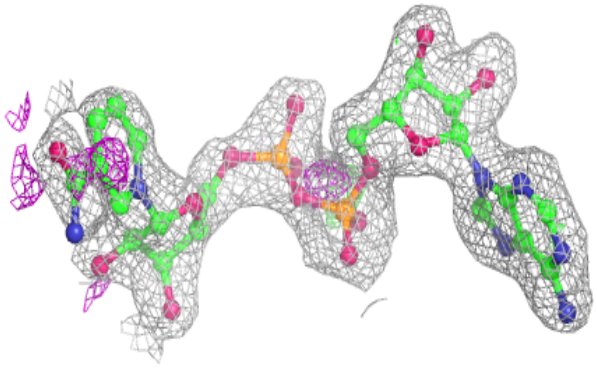


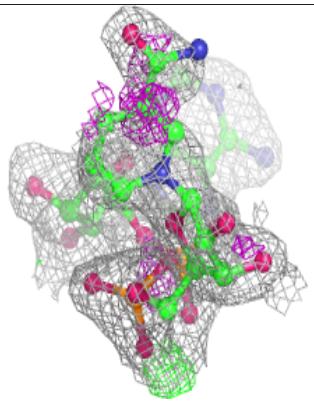


Electron density around NAD D 601:

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

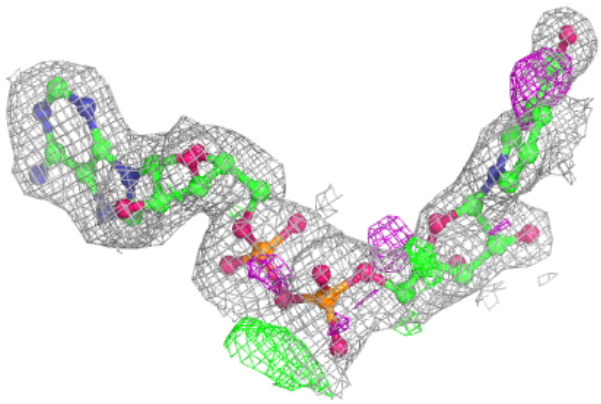


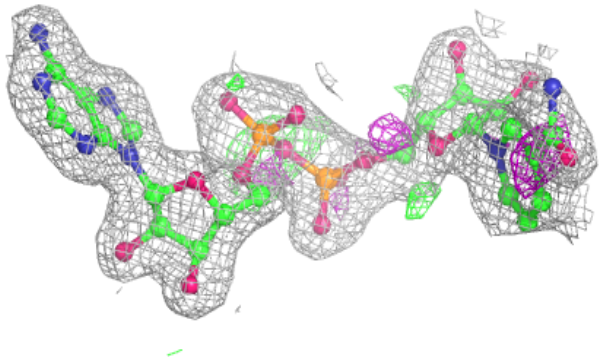


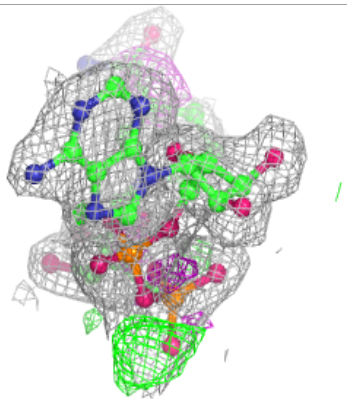


Electron density around NAD B 601:

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

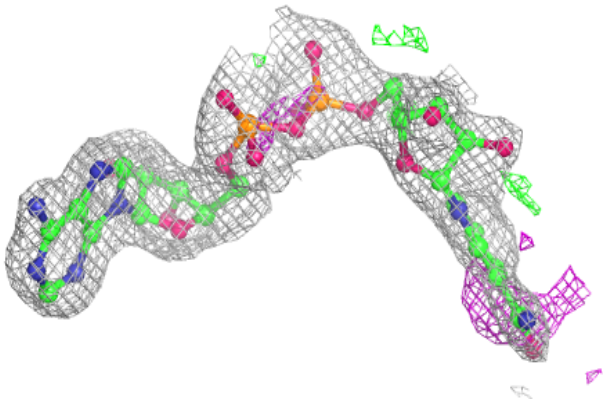


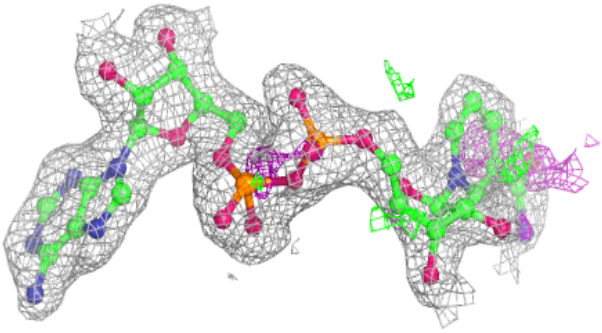


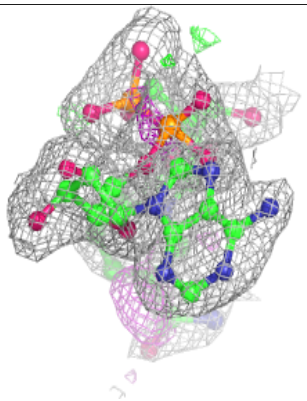


Electron density around NAD A 601:

$2mF_o$-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.