Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 04:54 pm BST

PDB ID	:	2WDZ
Title	:	Crystal structure of the short chain dehydrogenase Galactitol- Dehydrogenase (GatDH) of Rhodobacter sphaeroides in complex with NAD+ and 1,2-Pentandiol
Authors	:	Carius, Y.; Christian, H.; Faust, A.; Kornberger, P.; Kohring, G.W.; Giffhorn, F.; Scheidig, A.J.
Deposited on	:	2009-03-27
Resolution	:	1.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

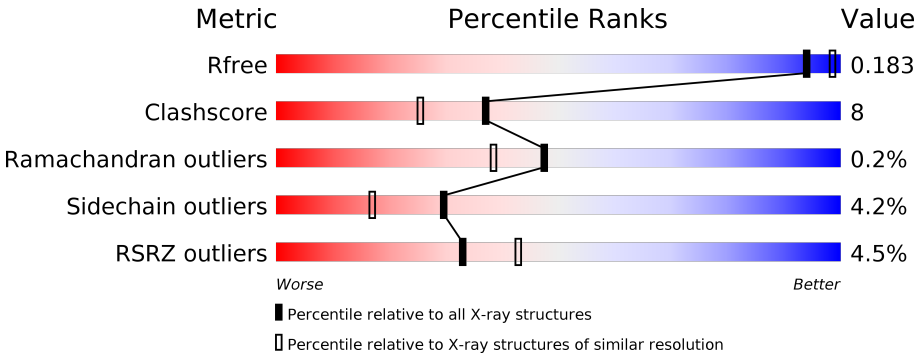
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	254	3% 88% 9% .
1	B	254	5% 85% 14% .
1	C	254	6% 84% 15% .
1	D	254	4% 84% 13% .

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	1SP	A	258	-	-	-	X
4	1SP	A	259	-	-	X	-
4	1SP	B	258	-	-	-	X
4	1SP	D	258	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8126 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 SHORT-CHAIN DEHYDROGENASE/REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	1	0
			1855	1159	334	348	14			
1	B	254	Total	C	N	O	S	0	0	0
			1847	1154	331	348	14			
1	C	254	Total	C	N	O	S	0	1	0
			1857	1159	335	349	14			
1	D	254	Total	C	N	O	S	0	1	0
			1857	1159	335	349	14			

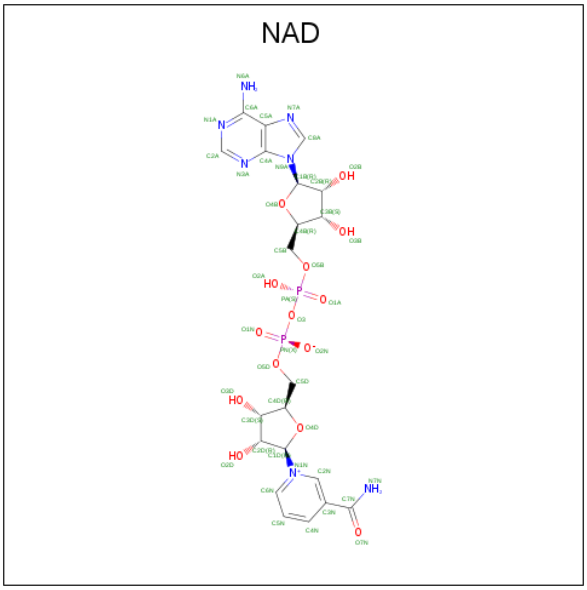
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	GLY	SEE REMARK 999	UNP Q3J3W2
B	45	ALA	GLY	SEE REMARK 999	UNP Q3J3W2
C	45	ALA	GLY	SEE REMARK 999	UNP Q3J3W2
D	45	ALA	GLY	SEE REMARK 999	UNP Q3J3W2
A	53	GLN	GLU	SEE REMARK 999	UNP Q3J3W2
B	53	GLN	GLU	SEE REMARK 999	UNP Q3J3W2
C	53	GLN	GLU	SEE REMARK 999	UNP Q3J3W2
D	53	GLN	GLU	SEE REMARK 999	UNP Q3J3W2
A	61	ALA	SER	SEE REMARK 999	UNP Q3J3W2
B	61	ALA	SER	SEE REMARK 999	UNP Q3J3W2
C	61	ALA	SER	SEE REMARK 999	UNP Q3J3W2
D	61	ALA	SER	SEE REMARK 999	UNP Q3J3W2
A	79	GLU	ALA	SEE REMARK 999	UNP Q3J3W2
B	79	GLU	ALA	SEE REMARK 999	UNP Q3J3W2
C	79	GLU	ALA	SEE REMARK 999	UNP Q3J3W2
D	79	GLU	ALA	SEE REMARK 999	UNP Q3J3W2
A	208	GLU	GLY	SEE REMARK 999	UNP Q3J3W2
B	208	GLU	GLY	SEE REMARK 999	UNP Q3J3W2
C	208	GLU	GLY	SEE REMARK 999	UNP Q3J3W2
D	208	GLU	GLY	SEE REMARK 999	UNP Q3J3W2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

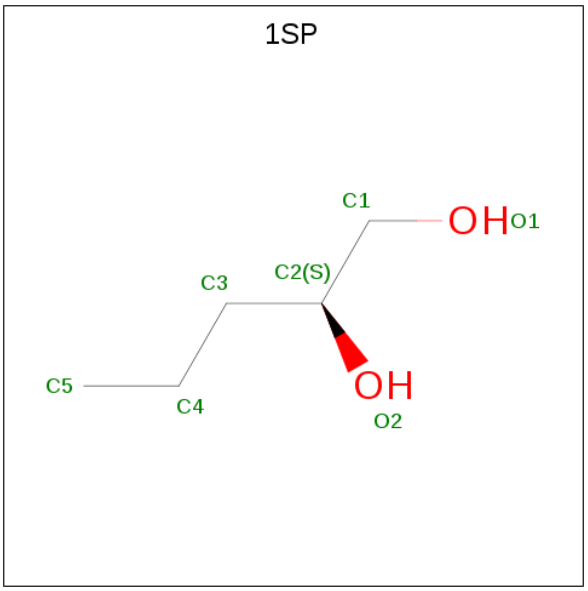
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is (2S)-pentane-1,2-diol (three-letter code: 1SP) (formula: $C_5H_{12}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 5 2	0	0
4	A	1	Total C O 7 5 2	0	0
4	B	1	Total C O 7 5 2	0	0
4	C	1	Total C O 7 5 2	0	0
4	D	1	Total C O 7 5 2	0	0

- Molecule 5 is water.

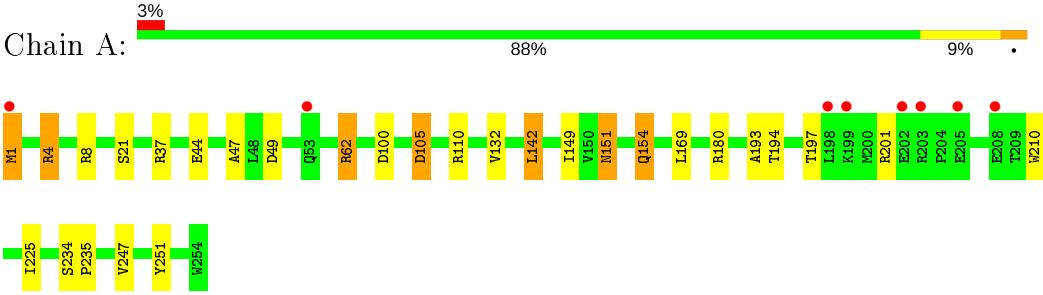
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0
5	B	119	Total O 119 119	0	0
5	C	108	Total O 108 108	0	0
5	D	118	Total O 118 118	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

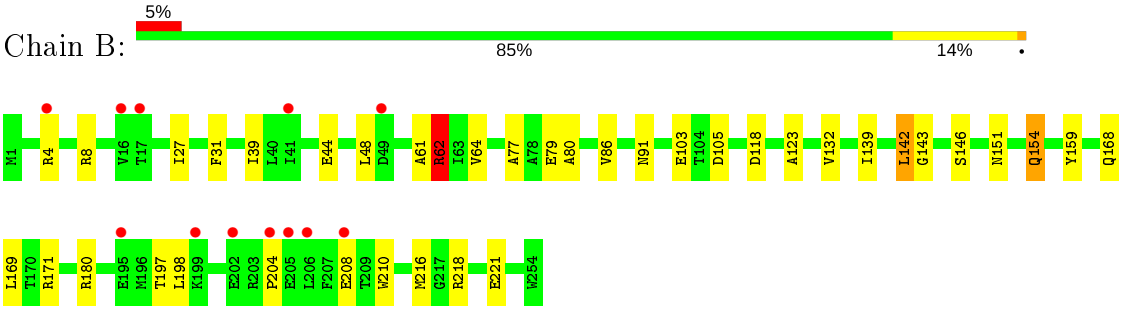
- Molecule 1: SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain A:



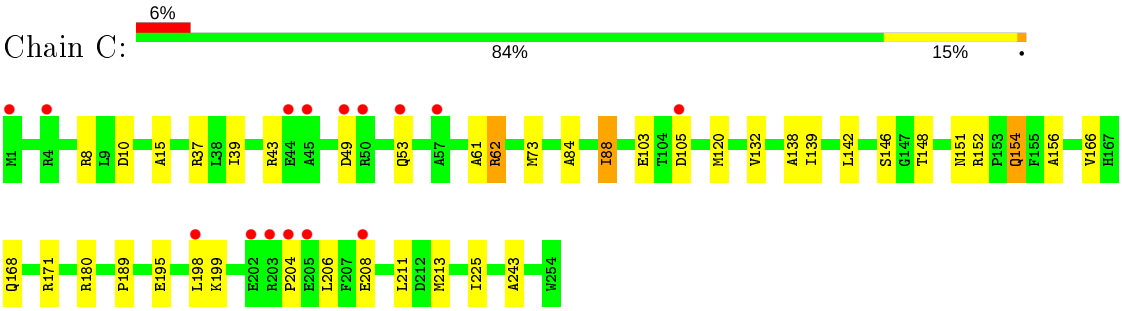
- Molecule 1: SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain B:



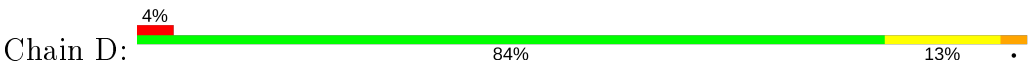
- Molecule 1: SHORT-CHAIN DEHYDROGENASE/REDUCTASE

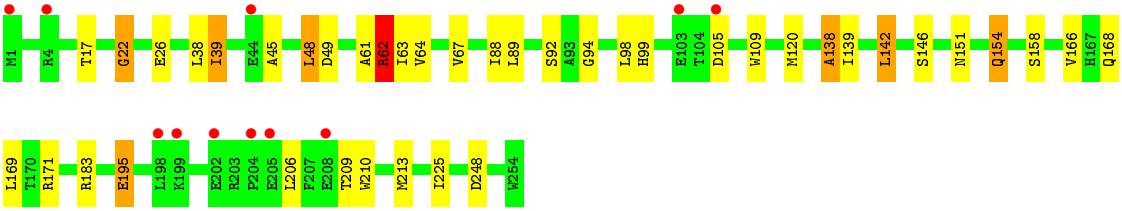
Chain C:



- Molecule 1: SHORT-CHAIN DEHYDROGENASE/REDUCTASE

Chain D:




M1
R4
T17
G22
E26
L38
I39
E44
A45
L48
D49
A61
R62
I63
V64
V67
I88
L89
S92
A93
G94
L98
H99
E103
T104
D105
W109
M120
A138
I139
L142
S146
N151
Q154
S158
V166
H167
Q168
L169
T170
R171
R183
E196
L198
K199
E202
R203
P204
E205
L206
P207
E208
T209
W210
M213
I225
D248
W254

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	60.72Å 113.62Å 256.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 1.95 19.87 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.86-1.95) 98.4 (19.87-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.240 0.185 , 0.183	Depositor DCC
R_{free} test set	3240 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8126	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1SP, 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	0.98	1/1888 (0.1%)	0.91	3/2564 (0.1%)
1	B	1.02	7/1877 (0.4%)	0.92	2/2550 (0.1%)
1	C	0.88	3/1887 (0.2%)	0.85	4/2563 (0.2%)
1	D	1.05	8/1887 (0.4%)	0.95	7/2563 (0.3%)
All	All	0.98	19/7539 (0.3%)	0.91	16/10240 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	ARG	C-N	-13.93	1.02	1.34
1	D	94	GLY	C-N	-11.47	1.07	1.34
1	D	22	GLY	C-N	-9.68	1.11	1.34
1	D	38	LEU	C-N	-7.90	1.15	1.34
1	C	148	THR	C-N	-7.11	1.17	1.34
1	B	79	GLU	CB-CG	-6.95	1.39	1.52
1	D	39	ILE	C-N	-6.41	1.19	1.34
1	B	139	ILE	C-N	-6.39	1.19	1.34
1	A	62	ARG	C-N	-6.18	1.19	1.34
1	D	26	GLU	C-N	-6.07	1.20	1.34
1	D	225	ILE	C-N	-6.05	1.20	1.34
1	B	62	ARG	C-N	-6.03	1.20	1.34
1	B	79	GLU	CD-OE2	-5.75	1.19	1.25
1	B	103	GLU	CB-CG	5.57	1.62	1.52
1	C	139	ILE	C-N	-5.44	1.21	1.34
1	B	221	GLU	CG-CD	5.37	1.60	1.51
1	C	88	ILE	C-N	-5.31	1.21	1.34
1	D	138	ALA	C-N	-5.31	1.21	1.34
1	B	79	GLU	CD-OE1	-5.10	1.20	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	ILE	O-C-N	-7.96	109.96	122.70
1	A	142	LEU	CA-CB-CG	-7.74	97.50	115.30
1	D	142	LEU	CA-CB-CG	-7.46	98.14	115.30
1	D	248	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	94	GLY	O-C-N	-6.53	112.26	122.70
1	B	142	LEU	CA-CB-CG	-6.44	100.49	115.30
1	D	94	GLY	C-N-CA	5.95	136.57	121.70
1	A	37	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	118	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	148	THR	C-N-CA	5.49	135.41	121.70
1	C	142	LEU	CA-CB-CG	-5.48	102.70	115.30
1	A	100	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	63	ILE	CA-C-N	5.28	128.82	117.20
1	C	148	THR	O-C-N	-5.20	114.37	122.70
1	D	183	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	C	243	ALA	O-C-N	5.14	130.92	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1855	0	1847	32	0
1	B	1847	0	1834	30	0
1	C	1857	0	1840	25	0
1	D	1857	0	1835	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	2	0
3	C	44	0	26	2	0
3	D	44	0	26	0	0
4	A	14	0	24	19	0
4	B	7	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	7	0	12	0	0
4	D	7	0	12	0	0
5	A	150	0	0	5	1
5	B	119	0	0	1	1
5	C	108	0	0	0	0
5	D	118	0	0	1	1
All	All	8126	0	7520	118	2

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 8.

All (118) 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:49:ASP:HB2	4:A:259:1SP:H52C	1.40	1.02
1:C:152:ARG:HD3	1:C:213:MET:HE2	1.50	0.94
1:D:48:LEU:HD22	1:D:62:ARG:HG3	1.47	0.94
4:A:259:1SP:O1	1:D:62:ARG:NH1	2.02	0.92
1:A:44:GLU:HB2	5:A:2034:HOH:O	1.75	0.87
1:D:154:GLN:HE21	1:D:154:GLN:H	1.25	0.84
1:D:39:ILE:HD12	1:D:61:ALA:HB3	1.63	0.81
4:A:259:1SP:H12C	1:D:62:ARG:HD3	1.61	0.80
1:B:154:GLN:HE21	1:B:154:GLN:H	1.32	0.78
1:A:221:GLU:HG3	5:A:2127:HOH:O	1.84	0.76
1:C:189:PRO:HB3	1:C:225:ILE:HD12	1.68	0.75
1:A:49:ASP:HB2	4:A:259:1SP:C5	2.17	0.74
1:D:48:LEU:CD2	1:D:62:ARG:HG3	2.18	0.72
1:D:195:GLU:CD	1:D:195:GLU:H	1.93	0.72
1:A:8:ARG:NH1	1:B:4:ARG:HE	1.88	0.71
1:D:154:GLN:H	1:D:154:GLN:NE2	1.88	0.70
4:A:259:1SP:C1	1:D:62:ARG:HD3	2.24	0.67
4:A:259:1SP:H11C	1:D:49:ASP:N	2.10	0.66
1:B:169:LEU:HD23	1:B:169:LEU:C	2.16	0.66
1:B:39:ILE:HD12	1:B:61:ALA:HB3	1.78	0.65
1:A:154:GLN:HE22	1:A:210:TRP:HE1	1.45	0.65
1:C:154:GLN:H	1:C:154:GLN:HE21	1.45	0.65
1:C:152:ARG:HD3	1:C:213:MET:CE	2.24	0.65
1:C:152:ARG:HH11	1:C:213:MET:CE	2.12	0.63
1:C:154:GLN:H	1:C:154:GLN:NE2	1.96	0.63
1:D:48:LEU:HD22	1:D:62:ARG:CG	2.26	0.63
1:A:62:ARG:HH11	4:A:259:1SP:H53C	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	1:A:1:MET:CE	2.29	0.61
1:A:110[B]:ARG:HD2	5:A:2079:HOH:O	2.00	0.61
4:A:259:1SP:H1	1:D:62:ARG:HH11	1.42	0.61
4:A:259:1SP:H32C	1:D:64:VAL:HG21	1.83	0.61
1:B:154:GLN:HE22	1:B:210:TRP:HE1	1.48	0.60
1:B:154:GLN:NE2	1:B:154:GLN:H	1.96	0.60
1:A:62:ARG:HD2	4:A:259:1SP:H53C	1.84	0.60
1:A:1:MET:HA	1:A:1:MET:HE1	1.84	0.59
1:A:169:LEU:C	1:A:169:LEU:HD23	2.23	0.59
1:C:132:VAL:HG13	1:C:180:ARG:HD2	1.84	0.59
1:D:168:GLN:HE22	1:D:171:ARG:HE	1.52	0.58
4:A:259:1SP:HA	1:D:45:ALA:O	2.04	0.58
1:D:154:GLN:HE22	1:D:210:TRP:HE1	1.52	0.58
1:A:151:ASN:H	1:A:151:ASN:HD22	1.51	0.57
1:A:194:THR:O	1:A:201:ARG:NH2	2.37	0.56
1:A:225:ILE:HD13	1:A:247:VAL:HG11	1.87	0.56
1:C:204:PRO:O	1:C:208:GLU:HB2	2.06	0.56
1:C:152:ARG:HH11	1:C:213:MET:HE1	1.71	0.55
1:A:49:ASP:N	4:A:259:1SP:H51C	2.22	0.55
1:B:48:LEU:HD13	1:B:62:ARG:HG2	1.87	0.55
1:C:152:ARG:CD	1:C:213:MET:HE2	2.33	0.53
1:C:73:MET:HA	1:C:73:MET:CE	2.37	0.53
1:B:80:ALA:HB1	1:B:86:VAL:HG21	1.91	0.53
1:A:62:ARG:CD	4:A:259:1SP:H53C	2.38	0.53
1:B:169:LEU:O	1:B:169:LEU:HD23	2.09	0.53
1:C:37:ARG:NH2	1:C:84:ALA:HB2	2.23	0.52
1:B:204:PRO:O	1:B:208:GLU:HG3	2.09	0.52
1:B:48:LEU:HD13	1:B:62:ARG:CG	2.40	0.52
1:C:146:SER:OG	1:C:151:ASN:ND2	2.38	0.52
4:A:259:1SP:HA	1:D:45:ALA:CA	2.40	0.51
1:D:89:LEU:HB3	1:D:139:ILE:HG12	1.92	0.51
1:B:159:TYR:CE2	4:B:258:1SP:H11C	2.46	0.51
1:B:48:LEU:HD12	1:B:64:VAL:HG22	1.94	0.50
1:D:209:THR:O	1:D:213:MET:HG2	2.12	0.50
1:D:120:MET:SD	1:D:166:VAL:HG13	2.52	0.49
4:A:259:1SP:C2	1:D:45:ALA:O	2.60	0.49
1:A:225:ILE:HD13	1:A:247:VAL:CG1	2.43	0.48
1:D:146:SER:OG	1:D:151:ASN:ND2	2.44	0.48
1:B:146:SER:OG	1:B:151:ASN:ND2	2.37	0.48
1:A:154:GLN:H	1:A:154:GLN:NE2	2.11	0.48
1:A:4:ARG:HB2	1:A:4:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLN:HE22	1:C:171:ARG:HE	1.62	0.47
1:C:39:ILE:HD12	1:C:61:ALA:HB3	1.97	0.47
1:B:151:ASN:H	1:B:151:ASN:HD22	1.63	0.47
1:B:216:MET:HE1	1:B:218:ARG:NH2	2.30	0.46
1:B:105:ASP:HB2	5:B:2058:HOH:O	2.14	0.46
4:A:259:1SP:H11C	1:D:49:ASP:CA	2.46	0.46
1:D:39:ILE:CD1	1:D:61:ALA:HB3	2.40	0.46
1:B:91:ASN:HD21	1:B:123:ALA:HB3	1.81	0.46
1:B:168:GLN:HE22	1:B:171:ARG:HE	1.64	0.46
1:C:189:PRO:HB3	1:C:225:ILE:CD1	2.42	0.45
1:A:44:GLU:HG2	1:A:47:ALA:H	1.82	0.45
1:A:197:THR:HG21	3:A:257:NAD:H72N	1.80	0.45
4:A:259:1SP:C1	1:D:62:ARG:HH11	2.23	0.45
1:D:17:THR:O	1:D:92:SER:HB3	2.16	0.45
1:A:8:ARG:NH1	1:B:4:ARG:NE	2.62	0.45
5:A:2007:HOH:O	1:B:8:ARG:HD3	2.17	0.45
3:C:257:NAD:O1A	1:D:195:GLU:HG2	2.16	0.44
1:D:98:LEU:O	1:D:99:HIS:HB3	2.17	0.44
1:B:143:GLY:O	3:B:257:NAD:H6N	2.17	0.44
1:A:132:VAL:HG13	1:A:180:ARG:HD2	1.99	0.44
1:A:44:GLU:CB	5:A:2034:HOH:O	2.51	0.44
1:C:195:GLU:HG2	5:D:2115:HOH:O	2.16	0.44
1:D:22:GLY:HA2	1:D:195:GLU:OE1	2.16	0.44
1:A:105:ASP:N	1:A:105:ASP:OD1	2.49	0.43
1:A:149:ILE:HD13	1:A:251:TYR:HE2	1.84	0.43
1:B:151:ASN:H	1:B:151:ASN:ND2	2.16	0.43
1:D:88:ILE:HA	1:D:138:ALA:O	2.19	0.43
1:B:197:THR:HG21	3:B:257:NAD:H72N	1.84	0.43
1:C:88:ILE:HA	1:C:138:ALA:O	2.18	0.43
1:D:109:TRP:CE3	1:D:158:SER:HB3	2.54	0.43
1:C:120:MET:SD	1:C:166:VAL:HG13	2.59	0.42
1:C:198:LEU:HD23	1:C:199:LYS:CE	2.49	0.42
4:A:259:1SP:HA	1:D:45:ALA:C	2.39	0.42
3:C:257:NAD:C6A	1:D:67:VAL:HG22	2.50	0.42
1:A:234:SER:HB2	1:A:235:PRO:HD2	2.02	0.42
1:B:169:LEU:CD2	1:B:169:LEU:C	2.87	0.42
1:A:151:ASN:N	1:A:151:ASN:HD22	2.17	0.42
1:B:77:ALA:O	1:B:80:ALA:HB3	2.20	0.42
1:C:49:ASP:HA	1:C:62:ARG:NH1	2.35	0.42
1:C:152:ARG:NH1	1:C:213:MET:CE	2.83	0.41
1:A:151:ASN:N	1:A:151:ASN:ND2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG13	1:B:180:ARG:HD2	2.02	0.41
1:C:15:ALA:HA	1:C:39:ILE:HB	2.01	0.41
1:C:8:ARG:HB3	1:C:10:ASP:OD2	2.20	0.41
4:A:259:1SP:HA	1:D:45:ALA:HA	2.02	0.41
1:C:73:MET:HA	1:C:73:MET:HE1	2.01	0.41
1:A:4:ARG:HG2	1:B:8:ARG:HH11	1.85	0.41
1:A:8:ARG:HH12	1:B:4:ARG:HE	1.67	0.41
1:B:27:ILE:HG23	1:B:31:PHE:CE1	2.56	0.40
1:D:154:GLN:NE2	1:D:210:TRP:HE1	2.17	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:2103:HOH:O	5:D:2106:HOH:O[3_555]	1.61	0.59
5:A:2098:HOH:O	5:B:2080:HOH:O[4_555]	2.11	0.09

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	253/254 (100%)	247 (98%)	5 (2%)	1 (0%)	34 22
1	B	252/254 (99%)	247 (98%)	5 (2%)	0	100 100
1	C	253/254 (100%)	245 (97%)	7 (3%)	1 (0%)	34 22
1	D	253/254 (100%)	240 (95%)	13 (5%)	0	100 100
All	All	1011/1016 (100%)	979 (97%)	30 (3%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	C	156	ALA

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	174/174 (100%)	166 (95%)	8 (5%)	27	14
1	B	173/174 (99%)	168 (97%)	5 (3%)	42	31
1	C	173/174 (99%)	165 (95%)	8 (5%)	27	14
1	D	173/174 (99%)	165 (95%)	8 (5%)	27	14
All	All	693/696 (100%)	664 (96%)	29 (4%)	30	17

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG
1	A	21	SER
1	A	105	ASP
1	A	142	LEU
1	A	151	ASN
1	A	154	GLN
1	A	212	ASP
1	B	44	GLU
1	B	62	ARG
1	B	142	LEU
1	B	154	GLN
1	B	198	LEU
1	C	43	ARG
1	C	53	GLN
1	C	62	ARG
1	C	103	GLU
1	C	105	ASP
1	C	154	GLN
1	C	206	LEU

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Mol	Chain	Res	Type
1	C	211	LEU
1	D	48	LEU
1	D	62	ARG
1	D	105	ASP
1	D	142	LEU
1	D	154	GLN
1	D	169	LEU
1	D	195	GLU
1	D	206	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	151	ASN
1	A	154	GLN
1	B	91	ASN
1	B	151	ASN
1	B	154	GLN
1	B	168	GLN
1	C	53	GLN
1	C	91	ASN
1	C	151	ASN
1	C	154	GLN
1	C	168	GLN
1	D	91	ASN
1	D	151	ASN
1	D	154	GLN
1	D	168	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	NAD	D	257	-	42,48,48	1.97	6 (14%)	50,73,73	1.47	9 (18%)
3	NAD	B	257	-	42,48,48	2.05	8 (19%)	50,73,73	1.69	12 (24%)
4	1SP	D	258	-	6,6,6	0.96	0	4,6,6	0.51	0
4	1SP	C	258	-	6,6,6	0.68	0	4,6,6	0.78	0
4	1SP	A	258	-	6,6,6	0.66	0	4,6,6	0.54	0
3	NAD	A	257	-	42,48,48	2.24	5 (11%)	50,73,73	1.50	7 (14%)
4	1SP	B	258	-	6,6,6	0.59	0	4,6,6	0.44	0
3	NAD	C	257	-	42,48,48	1.99	8 (19%)	50,73,73	1.49	7 (14%)
4	1SP	A	259	-	6,6,6	0.97	1 (16%)	4,6,6	1.54	1 (25%)

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	257	-	-	4/26/62/62	0/5/5/5
3	NAD	B	257	-	-	5/26/62/62	0/5/5/5
4	1SP	D	258	-	-	2/5/5/5	-
4	1SP	C	258	-	-	2/5/5/5	-
4	1SP	A	258	-	-	4/5/5/5	-
3	NAD	A	257	-	-	4/26/62/62	0/5/5/5
4	1SP	B	258	-	-	5/5/5/5	-
3	NAD	C	257	-	-	4/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1SP	A	259	-	-	3/5/5/5	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	257	NAD	C2N-N1N	10.72	1.48	1.35
3	D	257	NAD	C2N-N1N	7.47	1.44	1.35
3	D	257	NAD	O7N-C7N	7.39	1.38	1.24
3	B	257	NAD	O7N-C7N	7.11	1.37	1.24
3	C	257	NAD	C2N-N1N	6.85	1.43	1.35
3	C	257	NAD	O7N-C7N	6.67	1.36	1.24
3	A	257	NAD	O7N-C7N	6.35	1.36	1.24
3	B	257	NAD	O4D-C1D	5.36	1.48	1.41
3	B	257	NAD	O4B-C1B	5.05	1.48	1.41
3	B	257	NAD	C2N-N1N	4.69	1.40	1.35
3	A	257	NAD	O4D-C1D	3.73	1.46	1.41
3	C	257	NAD	O4D-C1D	3.72	1.46	1.41
3	D	257	NAD	O4B-C1B	3.65	1.46	1.41
3	C	257	NAD	O4B-C1B	3.11	1.45	1.41
3	A	257	NAD	O4B-C1B	2.99	1.45	1.41
3	B	257	NAD	O4D-C4D	2.94	1.51	1.45
3	C	257	NAD	C3N-C7N	2.85	1.54	1.50
3	C	257	NAD	C2D-C1D	2.76	1.57	1.53
3	D	257	NAD	C6N-N1N	2.44	1.41	1.35
3	C	257	NAD	C6N-N1N	2.31	1.41	1.35
3	B	257	NAD	O4B-C4B	2.23	1.50	1.45
3	C	257	NAD	PN-O5D	2.18	1.68	1.59
3	B	257	NAD	C7N-N7N	2.16	1.37	1.33
3	B	257	NAD	PN-O2N	-2.14	1.45	1.55
3	D	257	NAD	PN-O5D	2.11	1.67	1.59
3	A	257	NAD	C4A-N3A	2.10	1.38	1.35
3	D	257	NAD	C2B-C1B	2.06	1.56	1.53
4	A	259	1SP	O2-C2	2.01	1.49	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	257	NAD	N3A-C2A-N1A	-5.51	120.06	128.68
3	A	257	NAD	N3A-C2A-N1A	-4.71	121.32	128.68
3	B	257	NAD	C1B-N9A-C4A	-4.42	118.88	126.64
3	B	257	NAD	N3A-C2A-N1A	-4.29	121.97	128.68
3	D	257	NAD	N3A-C2A-N1A	-4.00	122.43	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	257	NAD	C6N-N1N-C2N	-3.41	118.87	121.97
3	C	257	NAD	O7N-C7N-C3N	3.32	123.61	119.63
3	D	257	NAD	C6N-N1N-C2N	-3.13	119.12	121.97
3	B	257	NAD	C2N-C3N-C4N	3.06	121.72	118.26
3	B	257	NAD	O5D-PN-O1N	2.97	120.66	109.07
3	A	257	NAD	O2N-PN-O1N	2.89	126.55	112.24
3	C	257	NAD	C6N-N1N-C2N	-2.89	119.34	121.97
3	D	257	NAD	C2N-C3N-C4N	2.87	121.52	118.26
4	A	259	1SP	O2-C2-C3	2.76	117.10	109.21
3	B	257	NAD	C4A-C5A-N7A	-2.72	106.56	109.40
3	A	257	NAD	O5D-PN-O1N	2.66	119.45	109.07
3	C	257	NAD	O5D-PN-O1N	2.62	119.32	109.07
3	B	257	NAD	O7N-C7N-N7N	2.58	126.24	122.58
3	A	257	NAD	C2A-N1A-C6A	2.56	123.14	118.75
3	D	257	NAD	O5D-PN-O1N	2.51	118.89	109.07
3	D	257	NAD	O4D-C1D-C2D	-2.51	103.25	106.93
3	C	257	NAD	C2A-N1A-C6A	2.40	122.87	118.75
3	D	257	NAD	O2N-PN-O1N	2.38	124.00	112.24
3	D	257	NAD	C3N-C7N-N7N	-2.35	114.93	117.75
3	B	257	NAD	O2A-PA-O1A	2.31	123.64	112.24
3	A	257	NAD	C5B-C4B-C3B	-2.30	106.55	115.18
3	B	257	NAD	C3N-C2N-N1N	-2.29	118.19	120.43
3	D	257	NAD	C2A-N1A-C6A	2.25	122.61	118.75
3	C	257	NAD	O2N-PN-O5D	2.25	118.20	107.75
3	B	257	NAD	O2N-PN-O1N	2.25	123.37	112.24
3	A	257	NAD	O2A-PA-O1A	2.19	123.06	112.24
3	B	257	NAD	O4B-C4B-C3B	2.15	109.36	105.11
3	D	257	NAD	C1B-N9A-C4A	-2.13	122.90	126.64
3	B	257	NAD	C6N-N1N-C2N	-2.11	120.05	121.97
3	B	257	NAD	C5D-C4D-C3D	-2.10	107.29	115.18
3	C	257	NAD	O2N-PN-O1N	2.06	122.42	112.24

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	257	NAD	O4D-C1D-N1N-C2N
3	B	257	NAD	C5D-O5D-PN-O1N
3	B	257	NAD	O4D-C1D-N1N-C2N
3	B	257	NAD	O4D-C1D-N1N-C6N
4	D	258	1SP	O1-C1-C2-C3
4	D	258	1SP	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	258	1SP	O2-C2-C3-C4
3	A	257	NAD	C5D-O5D-PN-O1N
3	A	257	NAD	O4D-C1D-N1N-C2N
4	B	258	1SP	O1-C1-C2-C3
3	C	257	NAD	C5D-O5D-PN-O3
3	C	257	NAD	O4D-C1D-N1N-C2N
4	A	259	1SP	C2-C3-C4-C5
4	C	258	1SP	O1-C1-C2-O2
4	B	258	1SP	O1-C1-C2-O2
4	A	258	1SP	C1-C2-C3-C4
4	B	258	1SP	O2-C2-C3-C4
4	B	258	1SP	C1-C2-C3-C4
4	B	258	1SP	C2-C3-C4-C5
4	C	258	1SP	O1-C1-C2-C3
4	A	258	1SP	O1-C1-C2-C3
4	A	259	1SP	C1-C2-C3-C4
4	A	259	1SP	O2-C2-C3-C4
3	B	257	NAD	C5D-O5D-PN-O3
3	A	257	NAD	C5D-O5D-PN-O3
3	C	257	NAD	C5D-O5D-PN-O2N
3	D	257	NAD	O4B-C4B-C5B-O5B
3	D	257	NAD	C5D-O5D-PN-O3
4	A	258	1SP	O1-C1-C2-O2
3	B	257	NAD	O4B-C4B-C5B-O5B
3	C	257	NAD	O4B-C4B-C5B-O5B
3	D	257	NAD	C5D-O5D-PN-O2N
3	A	257	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

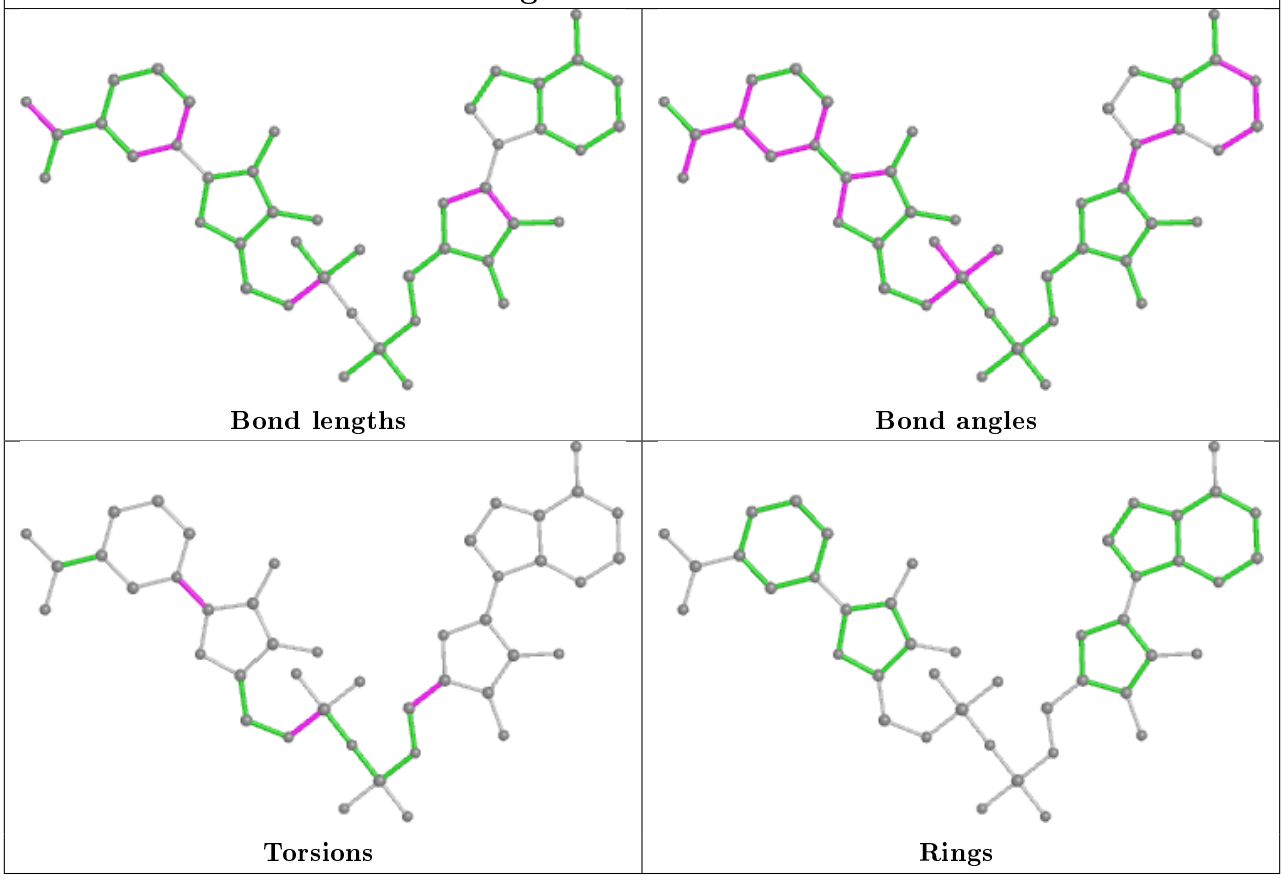
5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	257	NAD	2	0
3	A	257	NAD	1	0
4	B	258	1SP	1	0
3	C	257	NAD	2	0
4	A	259	1SP	19	0

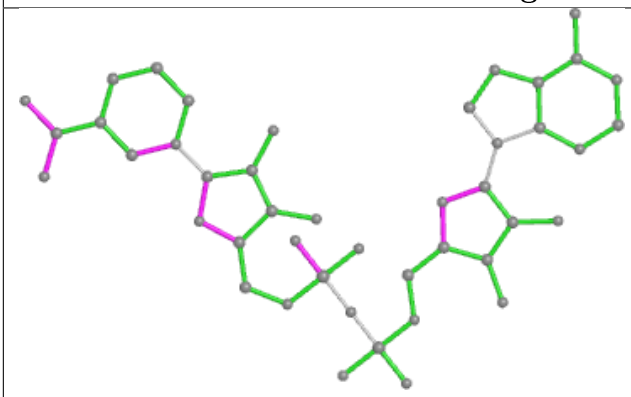
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

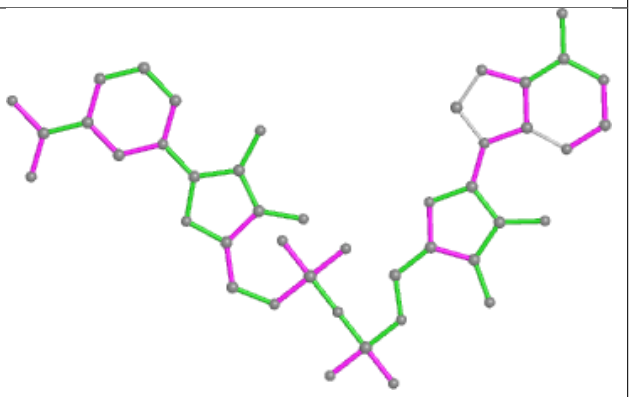
Ligand NAD D 257



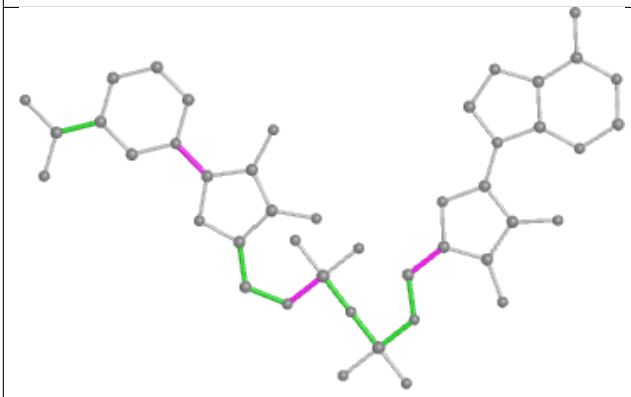
Ligand NAD B 257



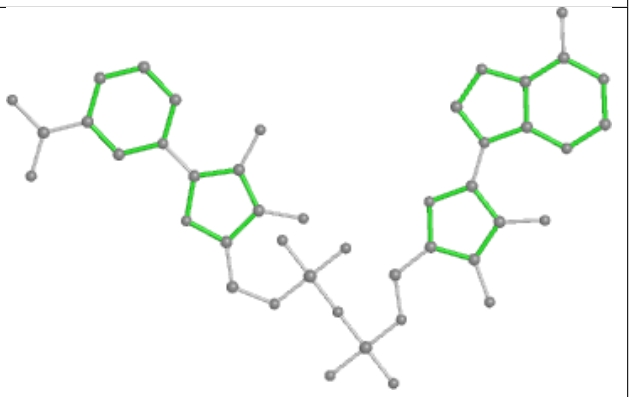
Bond lengths



Bond angles

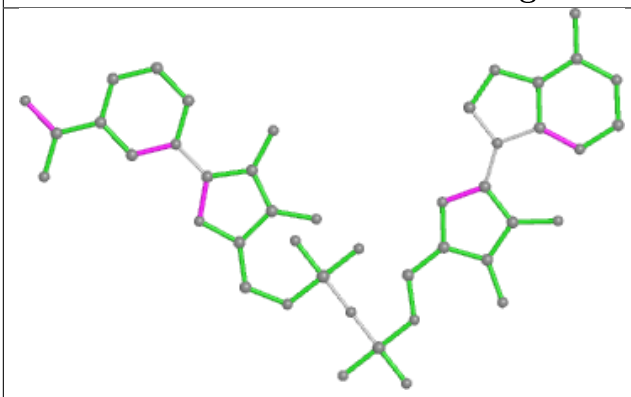


Torsions

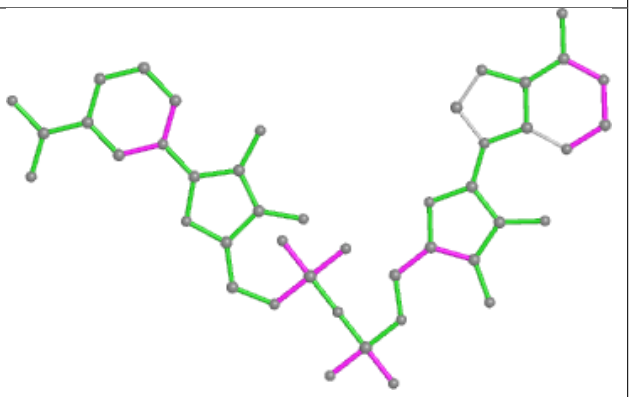


Rings

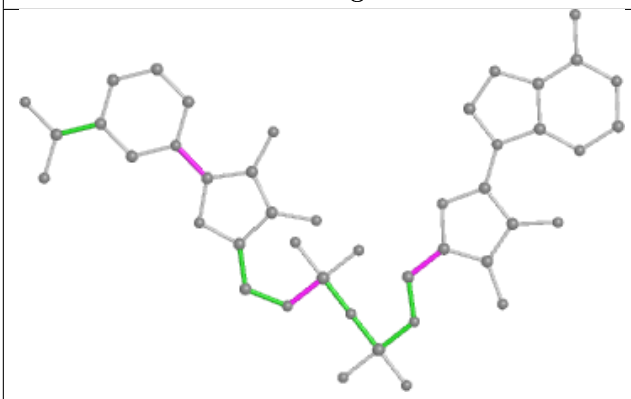
Ligand NAD A 257



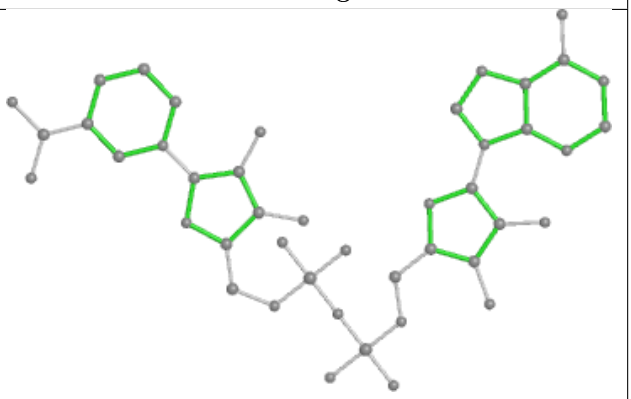
Bond lengths



Bond angles

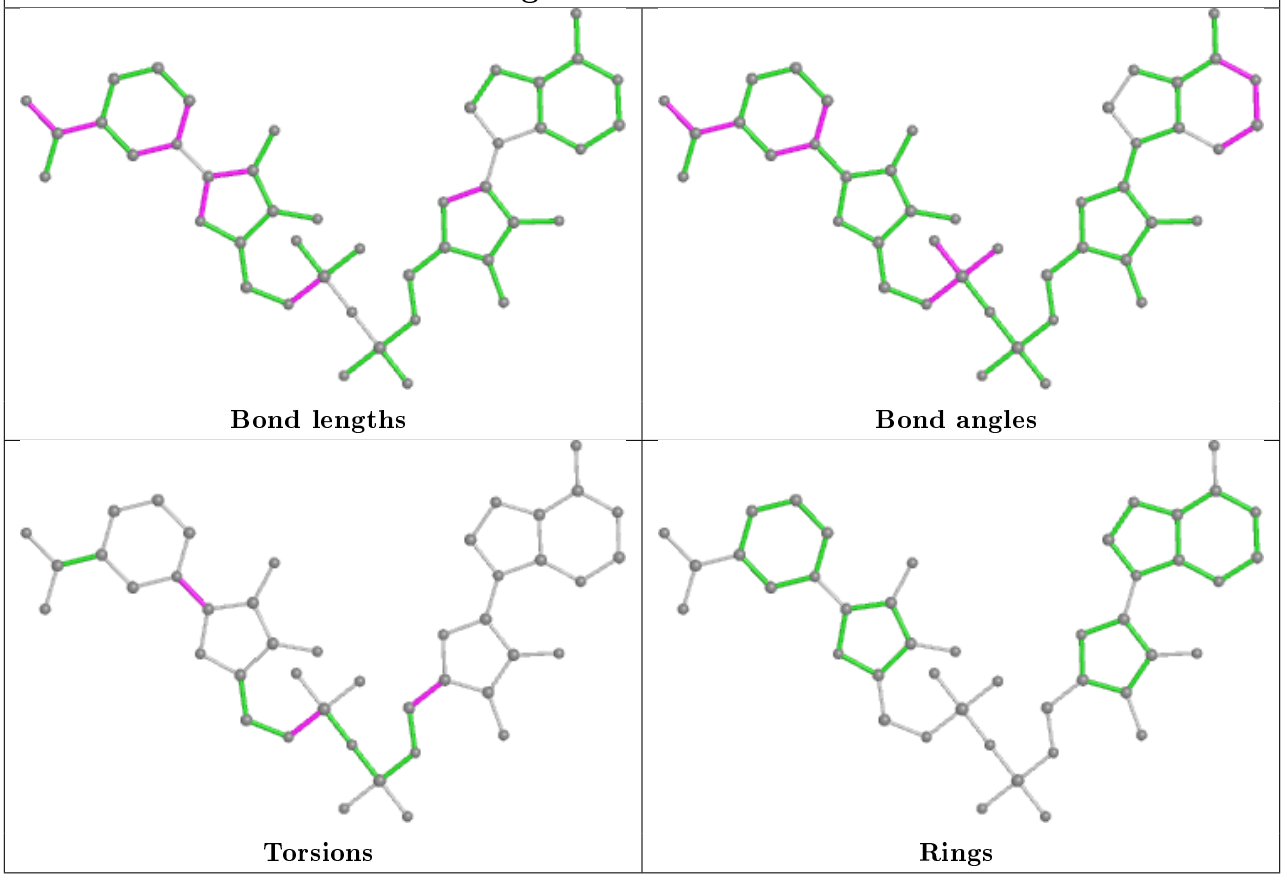


Torsions



Rings

Ligand NAD C 257



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	7
1	B	2
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	62:ARG	C	63:ILE	N	1.20
1	D	26:GLU	C	27:ILE	N	1.20
1	D	225:ILE	C	226:ALA	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	62:ARG	C	63:ILE	N	1.19
1	B	139:ILE	C	140:VAL	N	1.19
1	D	39:ILE	C	40:LEU	N	1.19
1	C	148:THR	C	149:ILE	N	1.17
1	D	38:LEU	C	39:ILE	N	1.15
1	D	22:GLY	C	23:ILE	N	1.11
1	D	94:GLY	C	95:ILE	N	1.07
1	D	62:ARG	C	63:ILE	N	1.02

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, 95^{th} 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	254/254 (100%)	-0.01	8 (3%)	49	58	12, 21, 42, 59	0
1	B	254/254 (100%)	0.11	12 (4%)	31	41	13, 22, 45, 60	0
1	C	254/254 (100%)	0.23	15 (5%)	22	30	17, 26, 51, 62	0
1	D	254/254 (100%)	0.13	11 (4%)	35	45	14, 23, 52, 67	0
All	All	1016/1016 (100%)	0.12	46 (4%)	33	43	12, 23, 48, 67	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	199	LYS	5.0
1	C	198	LEU	5.0
1	C	1	MET	4.9
1	D	204	PRO	4.6
1	D	208	GLU	4.1
1	D	198	LEU	4.0
1	A	205	GLU	3.8
1	C	57	ALA	3.7
1	D	202	GLU	3.7
1	C	4	ARG	3.6
1	D	205	GLU	3.5
1	A	199	LYS	3.3
1	A	198	LEU	3.3
1	B	199	LYS	3.2
1	B	205	GLU	3.1
1	B	204	PRO	2.9
1	A	1	MET	2.9
1	C	45	ALA	2.7
1	A	208	GLU	2.7
1	B	202	GLU	2.7
1	C	50	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	208	GLU	2.6
1	C	53	GLN	2.6
1	B	4	ARG	2.5
1	B	208	GLU	2.5
1	C	204	PRO	2.4
1	C	205	GLU	2.4
1	B	16	VAL	2.4
1	A	202	GLU	2.4
1	D	44	GLU	2.3
1	D	103	GLU	2.3
1	B	41	ILE	2.3
1	B	206	LEU	2.3
1	C	49	ASP	2.3
1	A	203	ARG	2.3
1	A	53	GLN	2.2
1	D	1	MET	2.2
1	C	44	GLU	2.2
1	C	105	ASP	2.2
1	B	195	GLU	2.1
1	D	105	ASP	2.1
1	B	17	THR	2.1
1	C	202	GLU	2.1
1	D	4	ARG	2.0
1	B	49	ASP	2.0
1	C	203	ARG	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 carbohydrates in this entry.

6.4 Ligands (i)

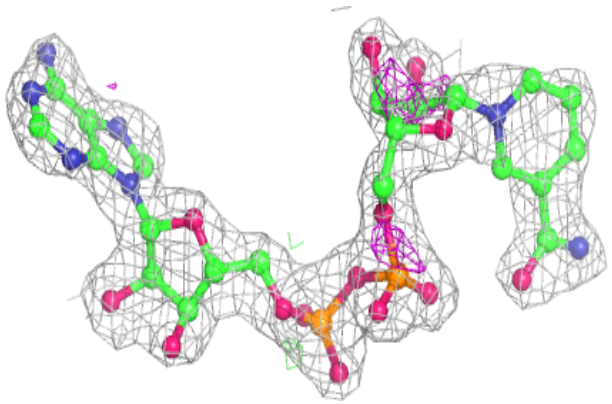
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

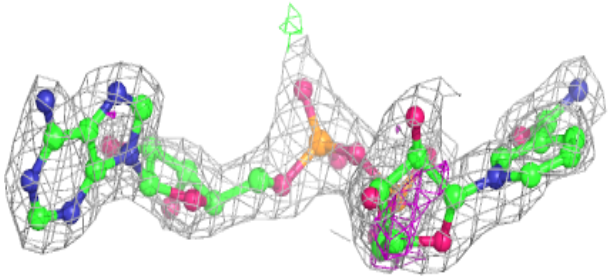
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1SP	D	258	7/7	0.67	0.52	53,56,58,58	0
4	1SP	B	258	7/7	0.67	0.48	47,52,53,56	0
4	1SP	C	258	7/7	0.69	0.39	55,57,58,59	0
4	1SP	A	258	7/7	0.75	0.54	62,64,64,66	0
4	1SP	A	259	7/7	0.77	0.25	31,37,43,44	0
3	NAD	C	257	44/44	0.92	0.16	32,39,42,43	0
3	NAD	B	257	44/44	0.95	0.09	19,25,28,32	0
3	NAD	A	257	44/44	0.96	0.09	20,24,27,30	0
3	NAD	D	257	44/44	0.97	0.08	24,29,33,33	0
2	MG	B	255	1/1	0.97	0.13	27,27,27,27	1
2	MG	A	255	1/1	0.98	0.07	25,25,25,25	1
2	MG	D	256	1/1	0.99	0.05	20,20,20,20	1
2	MG	C	256	1/1	0.99	0.05	20,20,20,20	1

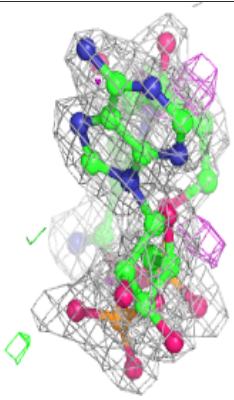
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 257:

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

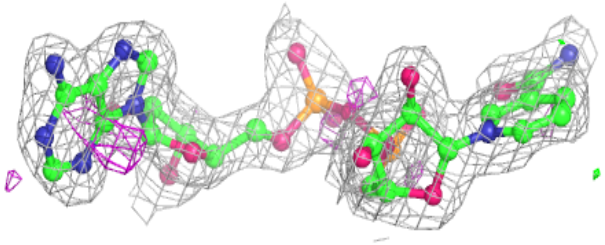


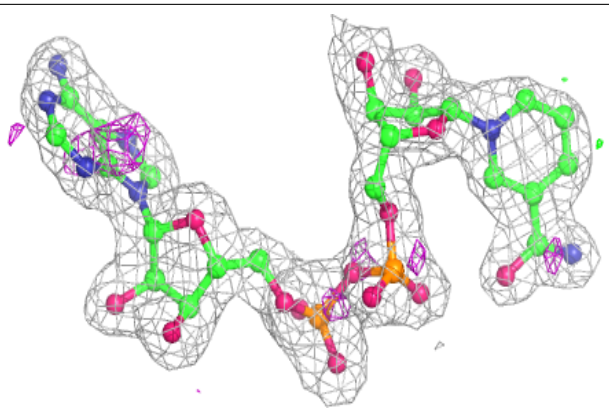


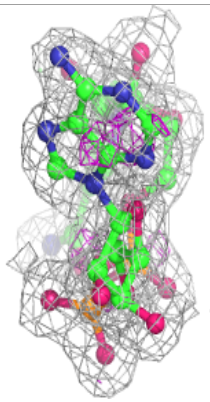


Electron density around NAD B 257:

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

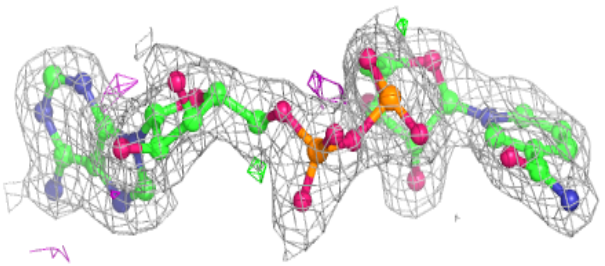


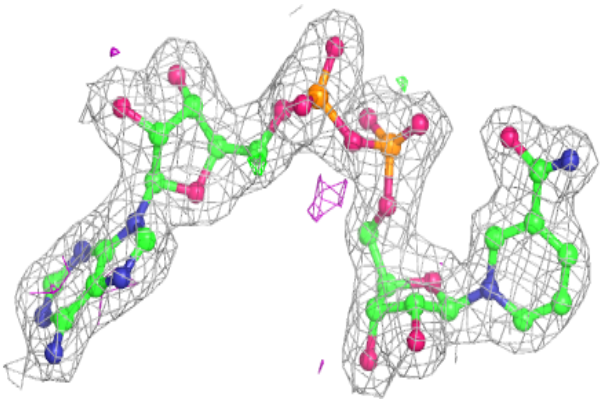


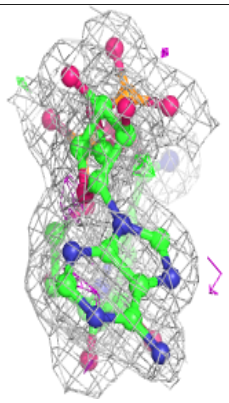


Electron density around NAD A 257:

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

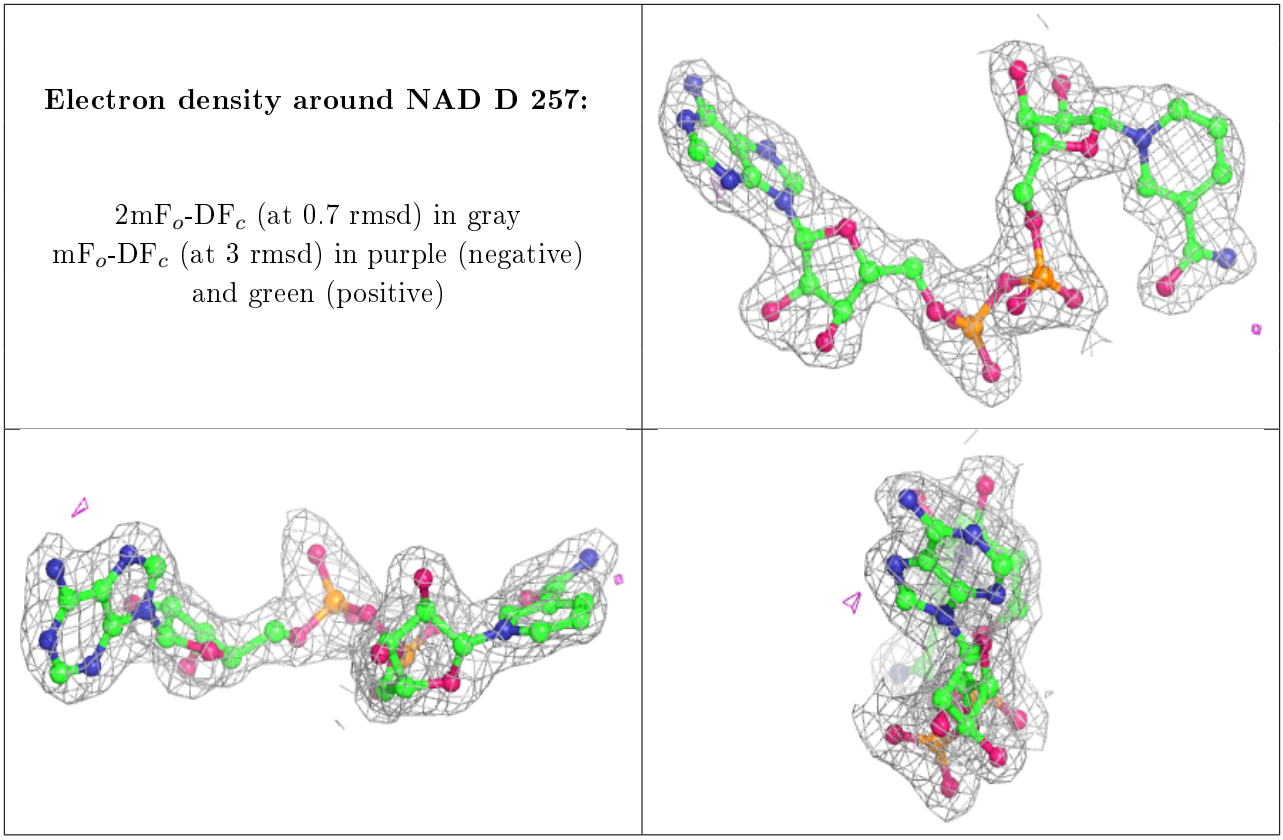






Electron density around NAD D 257:

$2mF_o$-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.