Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 09:52 PM EDT

PDB ID	:	5V8X
Title	:	Mutant Structures of Streptococcus Agalactiae GBS Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH)
Authors	:	Schormann, N.; Ulett, G.C.; Chattopadhyay, D.
Deposited on	:	2017-03-22
Resolution	:	2.95 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 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:

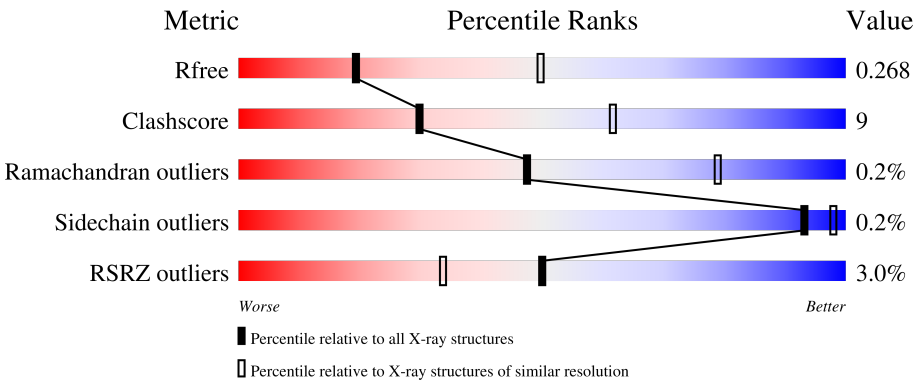
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	356	83% 10% • 6%
1	B	356	82% 12% 6%
1	C	356	4% 69% 22% • 8%
1	D	356	7% 75% 15% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10104 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2515	1569	439	499	8	0	0	0
1	B	334	2513	1568	438	499	8	0	0	0
1	C	329	2484	1551	433	492	8	0	0	0
1	D	319	2392	1486	417	481	8	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9ALW2
A	-18	GLY	-	expression tag	UNP Q9ALW2
A	-17	SER	-	expression tag	UNP Q9ALW2
A	-16	SER	-	expression tag	UNP Q9ALW2
A	-15	HIS	-	expression tag	UNP Q9ALW2
A	-14	HIS	-	expression tag	UNP Q9ALW2
A	-13	HIS	-	expression tag	UNP Q9ALW2
A	-12	HIS	-	expression tag	UNP Q9ALW2
A	-11	HIS	-	expression tag	UNP Q9ALW2
A	-10	HIS	-	expression tag	UNP Q9ALW2
A	-9	SER	-	expression tag	UNP Q9ALW2
A	-8	SER	-	expression tag	UNP Q9ALW2
A	-7	GLY	-	expression tag	UNP Q9ALW2
A	-6	LEU	-	expression tag	UNP Q9ALW2
A	-5	VAL	-	expression tag	UNP Q9ALW2
A	-4	PRO	-	expression tag	UNP Q9ALW2
A	-3	ARG	-	expression tag	UNP Q9ALW2
A	-2	GLY	-	expression tag	UNP Q9ALW2
A	-1	SER	-	expression tag	UNP Q9ALW2
A	0	HIS	-	expression tag	UNP Q9ALW2
A	288	HIS	TYR	engineered mutation	UNP Q9ALW2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	289	SER	GLY	engineered mutation	UNP Q9ALW2
B	-19	MET	-	expression tag	UNP Q9ALW2
B	-18	GLY	-	expression tag	UNP Q9ALW2
B	-17	SER	-	expression tag	UNP Q9ALW2
B	-16	SER	-	expression tag	UNP Q9ALW2
B	-15	HIS	-	expression tag	UNP Q9ALW2
B	-14	HIS	-	expression tag	UNP Q9ALW2
B	-13	HIS	-	expression tag	UNP Q9ALW2
B	-12	HIS	-	expression tag	UNP Q9ALW2
B	-11	HIS	-	expression tag	UNP Q9ALW2
B	-10	HIS	-	expression tag	UNP Q9ALW2
B	-9	SER	-	expression tag	UNP Q9ALW2
B	-8	SER	-	expression tag	UNP Q9ALW2
B	-7	GLY	-	expression tag	UNP Q9ALW2
B	-6	LEU	-	expression tag	UNP Q9ALW2
B	-5	VAL	-	expression tag	UNP Q9ALW2
B	-4	PRO	-	expression tag	UNP Q9ALW2
B	-3	ARG	-	expression tag	UNP Q9ALW2
B	-2	GLY	-	expression tag	UNP Q9ALW2
B	-1	SER	-	expression tag	UNP Q9ALW2
B	0	HIS	-	expression tag	UNP Q9ALW2
B	288	HIS	TYR	engineered mutation	UNP Q9ALW2
B	289	SER	GLY	engineered mutation	UNP Q9ALW2
C	-19	MET	-	expression tag	UNP Q9ALW2
C	-18	GLY	-	expression tag	UNP Q9ALW2
C	-17	SER	-	expression tag	UNP Q9ALW2
C	-16	SER	-	expression tag	UNP Q9ALW2
C	-15	HIS	-	expression tag	UNP Q9ALW2
C	-14	HIS	-	expression tag	UNP Q9ALW2
C	-13	HIS	-	expression tag	UNP Q9ALW2
C	-12	HIS	-	expression tag	UNP Q9ALW2
C	-11	HIS	-	expression tag	UNP Q9ALW2
C	-10	HIS	-	expression tag	UNP Q9ALW2
C	-9	SER	-	expression tag	UNP Q9ALW2
C	-8	SER	-	expression tag	UNP Q9ALW2
C	-7	GLY	-	expression tag	UNP Q9ALW2
C	-6	LEU	-	expression tag	UNP Q9ALW2
C	-5	VAL	-	expression tag	UNP Q9ALW2
C	-4	PRO	-	expression tag	UNP Q9ALW2
C	-3	ARG	-	expression tag	UNP Q9ALW2
C	-2	GLY	-	expression tag	UNP Q9ALW2
C	-1	SER	-	expression tag	UNP Q9ALW2

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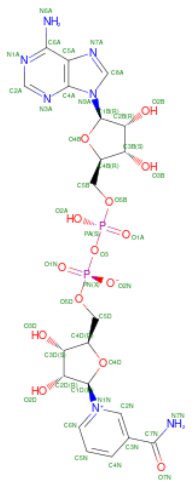
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q9ALW2
C	288	HIS	TYR	engineered mutation	UNP Q9ALW2
C	289	SER	GLY	engineered mutation	UNP Q9ALW2
D	-19	MET	-	expression tag	UNP Q9ALW2
D	-18	GLY	-	expression tag	UNP Q9ALW2
D	-17	SER	-	expression tag	UNP Q9ALW2
D	-16	SER	-	expression tag	UNP Q9ALW2
D	-15	HIS	-	expression tag	UNP Q9ALW2
D	-14	HIS	-	expression tag	UNP Q9ALW2
D	-13	HIS	-	expression tag	UNP Q9ALW2
D	-12	HIS	-	expression tag	UNP Q9ALW2
D	-11	HIS	-	expression tag	UNP Q9ALW2
D	-10	HIS	-	expression tag	UNP Q9ALW2
D	-9	SER	-	expression tag	UNP Q9ALW2
D	-8	SER	-	expression tag	UNP Q9ALW2
D	-7	GLY	-	expression tag	UNP Q9ALW2
D	-6	LEU	-	expression tag	UNP Q9ALW2
D	-5	VAL	-	expression tag	UNP Q9ALW2
D	-4	PRO	-	expression tag	UNP Q9ALW2
D	-3	ARG	-	expression tag	UNP Q9ALW2
D	-2	GLY	-	expression tag	UNP Q9ALW2
D	-1	SER	-	expression tag	UNP Q9ALW2
D	0	HIS	-	expression tag	UNP Q9ALW2
D	288	HIS	TYR	engineered mutation	UNP Q9ALW2
D	289	SER	GLY	engineered mutation	UNP Q9ALW2

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

NAD



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	6	6	6	0	0

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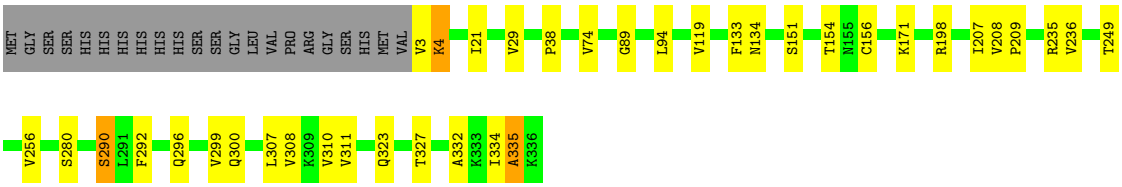
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	6	6	6	0	0
			Total	O		
4	C	2	2	2	0	0
			Total	O		
4	D	6	6	6	0	0

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.

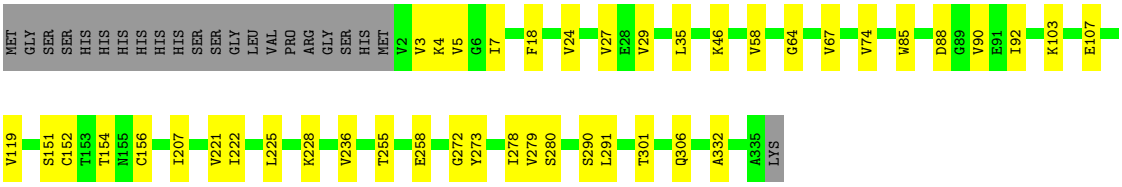
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



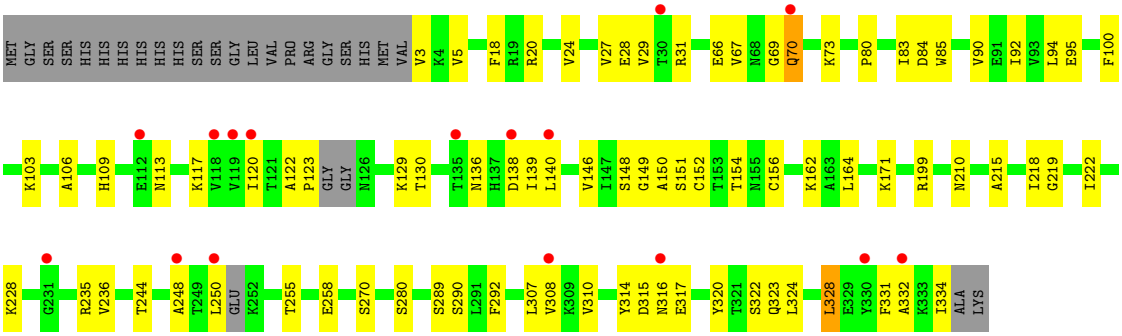
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain B:



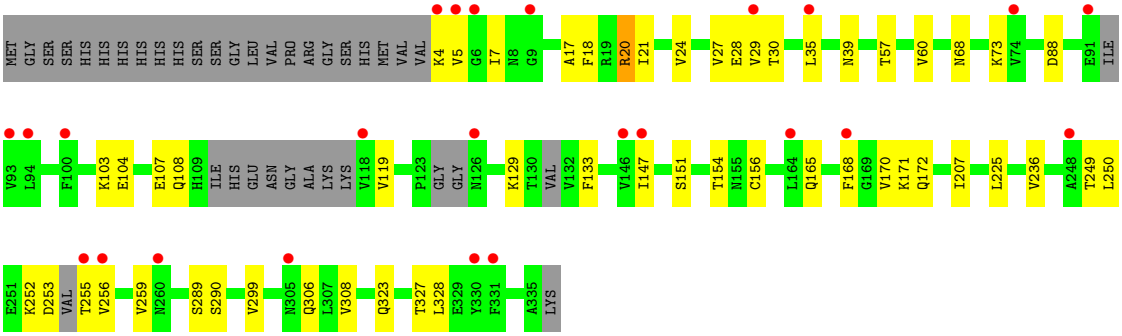
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain C:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain D:


MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
VAL
PRO
ARG
GLY
SER
HIS
MET
VAL
VAL
K4
V5
G6
I7
N8
G9
A17
F18
R19
R20
I21
V24
V27
E28
V29
T30
L35
N39
T57
V60
N68
K73
V74
D88
E91
ILE
V93
L94
F100
K103
E104
E107
Q108
H109
ILE
HIS
GLU
ASN
GLY
ALA
LYS
LYS
V118
V119
P123
GLY
GLY
N126
K129
T130
VAL
V132
F133
V146
I147
S151
T154
N155
C156
L164
Q165
F168
G169
V170
K171
Q172
I207
L225
V236
A248
T249
L250
E251
K252
D253
VAL
T255
V256
V259
N260
S289
S290
V299
N305
Q306
L307
V308
Q323
T327
L328
E329
Y330
F331
A335
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.10Å 107.81Å 91.43Å 90.00° 105.73° 90.00°	Depositor
Resolution (Å)	46.80 – 2.95 45.97 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.80-2.95) 99.2 (45.97-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.222 , 0.270 0.224 , 0.268	Depositor DCC
R_{free} test set	1298 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10104	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, MG

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	0.44	1/2553 (0.0%)	0.64	0/3464
1	B	0.43	0/2551	0.64	0/3463
1	C	0.45	0/2520	0.67	2/3418 (0.1%)
1	D	0.44	0/2422	0.65	0/3280
All	All	0.44	1/10046 (0.0%)	0.65	2/13625 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	SER	CB-OG	-5.17	1.35	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	328	LEU	CB-CG-CD2	5.59	120.50	111.00
1	C	235	ARG	NE-CZ-NH2	-5.57	117.52	120.30

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	2515	0	2496	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2513	0	2492	31	0
1	C	2484	0	2464	76	0
1	D	2392	0	2344	53	0
2	A	44	0	26	0	0
2	B	44	0	26	2	0
2	C	44	0	26	4	0
2	D	44	0	26	1	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	6	0	0	0	0
4	B	6	0	0	0	0
4	C	2	0	0	0	0
4	D	6	0	0	0	0
All	All	10104	0	9900	188	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 9.

All (188) 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:320:TYR:CE2	1:C:324:LEU:HD11	1.37	1.58
1:C:66:GLU:OE2	1:C:69:GLY:HA2	1.46	1.16
1:C:320:TYR:CE2	1:C:324:LEU:CD1	2.31	1.14
1:D:289:SER:OG	1:D:323:GLN:CG	2.17	0.92
1:C:18:PHE:CE2	1:C:29:VAL:HG11	2.07	0.89
1:C:320:TYR:CZ	1:C:324:LEU:HD11	2.07	0.89
1:C:320:TYR:HE2	1:C:324:LEU:HD11	1.34	0.83
1:C:316:ASN:OD1	1:C:317:GLU:N	2.13	0.81
1:C:20:ARG:NH1	1:C:322:SER:OG	2.16	0.79
1:C:316:ASN:OD1	1:C:317:GLU:HG3	1.83	0.77
1:C:320:TYR:CZ	1:C:324:LEU:HD21	2.20	0.76
1:A:300:GLN:HE21	1:A:307:LEU:HD12	1.50	0.76
1:A:300:GLN:NE2	1:A:307:LEU:HD12	1.99	0.76
1:D:171:LYS:HB2	1:D:249:THR:HG23	1.68	0.76
1:C:18:PHE:CD2	1:C:29:VAL:HG11	2.21	0.75
1:C:84:ASP:HB3	1:C:113:ASN:HD21	1.53	0.73
1:C:106:ALA:HB2	1:C:120:ILE:HD11	1.70	0.73
1:C:80:PRO:HA	1:C:83:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LYS:HE3	1:D:30:THR:CG2	2.19	0.71
1:D:24:VAL:HG13	1:D:27:VAL:CG1	2.21	0.71
1:D:289:SER:OG	1:D:323:GLN:HG3	1.89	0.70
1:A:198:ARG:NH1	1:B:278:ILE:O	2.25	0.70
1:D:24:VAL:CG1	1:D:27:VAL:CG1	2.71	0.68
1:D:4:LYS:HE3	1:D:30:THR:HG23	1.76	0.68
1:A:300:GLN:HG3	1:A:300:GLN:O	1.94	0.67
1:D:104:GLU:O	1:D:107:GLU:HG2	1.95	0.67
1:C:320:TYR:CD2	1:C:324:LEU:HD11	2.20	0.66
1:C:250:LEU:HD11	1:C:308:VAL:HG11	1.77	0.66
1:A:171:LYS:HD2	1:A:249:THR:HB	1.79	0.64
1:C:85:TRP:HB3	1:C:90:VAL:HG13	1.81	0.63
1:C:122:ALA:O	1:C:148:SER:OG	2.13	0.63
1:D:168:PHE:CD1	1:D:252:LYS:HD2	2.34	0.62
1:B:85:TRP:HB3	1:B:90:VAL:HG23	1.82	0.61
1:A:208:VAL:HG12	1:B:279:VAL:HG11	1.82	0.61
1:D:24:VAL:HG13	1:D:27:VAL:HG12	1.81	0.61
1:D:253:ASP:C	1:D:306:GLN:OE1	2.39	0.61
1:D:289:SER:OG	1:D:323:GLN:HG2	2.00	0.61
1:C:171:LYS:O	1:C:228:LYS:HD3	2.00	0.61
1:C:320:TYR:OH	1:C:324:LEU:HD21	2.00	0.60
1:C:80:PRO:HA	1:C:83:ILE:CD1	2.32	0.60
1:C:92:ILE:HD12	1:C:117:LYS:C	2.21	0.60
1:A:300:GLN:HE21	1:A:307:LEU:HB2	1.66	0.60
1:B:103:LYS:O	1:B:107:GLU:HG3	2.02	0.60
1:C:95:GLU:OE1	1:C:109:HIS:NE2	2.31	0.60
1:C:218:ILE:HD12	1:C:219:GLY:N	2.17	0.60
1:A:156:CYS:HA	1:A:290:SER:HB3	1.83	0.59
1:C:320:TYR:CD2	1:C:324:LEU:CD1	2.84	0.59
1:A:296:GLN:HB2	1:A:311:VAL:HG22	1.85	0.59
1:C:95:GLU:OE2	1:C:100:PHE:HD2	1.85	0.58
1:A:208:VAL:HG12	1:B:279:VAL:CG1	2.34	0.57
1:D:4:LYS:HB3	1:D:28:GLU:O	2.04	0.57
1:D:170:VAL:CG1	1:D:225:LEU:HD21	2.35	0.57
1:B:273:TYR:N	1:B:291:LEU:HD12	2.18	0.57
1:D:18:PHE:CD2	1:D:29:VAL:HG21	2.40	0.57
1:A:208:VAL:O	1:A:208:VAL:HG23	2.05	0.57
1:A:296:GLN:CD	1:A:311:VAL:HG21	2.26	0.56
1:C:129:LYS:HD3	1:C:139:ILE:CG2	2.35	0.56
1:C:162:LYS:HB2	1:C:222:ILE:CD1	2.35	0.56
1:B:151:SER:HG	1:B:154:THR:HG1	1.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:HB2	1:D:147:ILE:HG22	1.88	0.56
1:C:138:ASP:OD1	1:C:139:ILE:HD12	2.05	0.56
1:D:151:SER:HG	1:D:154:THR:HG1	1.50	0.56
1:C:84:ASP:HB3	1:C:113:ASN:ND2	2.21	0.55
1:B:156:CYS:HA	1:B:290:SER:HB2	1.88	0.55
1:D:156:CYS:HA	1:D:290:SER:HB2	1.89	0.55
1:C:18:PHE:CE2	1:C:29:VAL:CG1	2.87	0.55
1:C:156:CYS:HA	1:C:290:SER:HB2	1.88	0.55
1:D:170:VAL:HG11	1:D:225:LEU:HD21	1.89	0.55
1:C:199:ARG:HH11	1:C:210:ASN:HD21	1.53	0.54
1:D:289:SER:OG	1:D:323:GLN:CD	2.45	0.54
1:D:4:LYS:HE3	1:D:30:THR:HG21	1.89	0.54
1:A:256:VAL:HG23	1:A:299:VAL:HG22	1.90	0.53
1:C:250:LEU:HD11	1:C:308:VAL:CG1	2.39	0.53
1:C:140:LEU:HD23	1:C:331:PHE:CD1	2.43	0.53
1:D:5:VAL:HB	1:D:29:VAL:HG12	1.90	0.53
1:D:24:VAL:HG11	1:D:27:VAL:CG1	2.39	0.53
1:B:18:PHE:CD2	1:B:29:VAL:HG11	2.44	0.53
1:D:35:LEU:HD21	2:D:401:NAD:C6A	2.39	0.53
1:D:5:VAL:HG21	1:D:328:LEU:HD21	1.91	0.52
1:D:7:ILE:HD11	1:D:29:VAL:HG11	1.92	0.52
1:D:39:ASN:HA	1:D:60:VAL:HG11	1.91	0.52
1:A:21:ILE:HG21	1:A:29:VAL:HG23	1.92	0.51
1:A:151:SER:HG	1:A:154:THR:HG1	1.52	0.51
1:C:162:LYS:HD2	1:C:222:ILE:CD1	2.41	0.51
1:D:299:VAL:HG12	1:D:308:VAL:HG22	1.93	0.51
1:D:21:ILE:HG21	1:D:29:VAL:HG13	1.93	0.51
1:A:334:ILE:O	1:A:335:ALA:O	2.29	0.51
1:A:208:VAL:CG2	1:A:235:ARG:HB2	2.41	0.51
1:A:133:PHE:CD2	1:A:134:ASN:OD1	2.64	0.51
1:C:67:VAL:HG23	1:C:67:VAL:O	2.11	0.51
1:C:149:GLY:HA3	1:C:324:LEU:CD2	2.41	0.50
1:C:255:THR:HG22	1:C:258:GLU:HG3	1.93	0.50
1:A:280:SER:HB3	1:B:207:ILE:HB	1.94	0.50
1:D:20:ARG:HH11	1:D:20:ARG:HB3	1.76	0.50
1:C:140:LEU:HD23	1:C:331:PHE:HD1	1.77	0.50
1:D:170:VAL:HA	1:D:250:LEU:HA	1.93	0.50
1:C:151:SER:OG	1:C:154:THR:HG23	2.12	0.49
1:C:152:CYS:HB3	2:C:401:NAD:H4N	1.94	0.49
1:B:67:VAL:O	1:B:67:VAL:HG23	2.13	0.49
2:C:401:NAD:O1N	2:C:401:NAD:N7N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HB	1:B:280:SER:HB3	1.95	0.49
1:A:4:LYS:H	1:A:4:LYS:HD2	1.76	0.49
1:A:151:SER:OG	1:A:154:THR:OG1	2.24	0.48
1:C:152:CYS:H	2:C:401:NAD:H5N	1.78	0.48
1:B:272:GLY:C	1:B:291:LEU:HD12	2.33	0.48
1:D:165:GLN:HG2	1:D:170:VAL:HG12	1.94	0.48
1:D:24:VAL:CG1	1:D:27:VAL:HG12	2.43	0.48
1:D:108:GLN:HG2	1:D:108:GLN:O	2.13	0.48
1:C:215:ALA:O	1:C:218:ILE:HG13	2.14	0.47
1:C:106:ALA:CB	1:C:120:ILE:HD11	2.42	0.47
1:B:152:CYS:HB3	2:B:401:NAD:H4N	1.96	0.47
1:C:199:ARG:NH1	1:C:210:ASN:HD21	2.12	0.47
1:D:17:ALA:O	1:D:21:ILE:HG12	2.15	0.47
1:D:119:VAL:HG13	1:D:147:ILE:HD12	1.95	0.47
1:C:244:THR:HG23	1:C:314:TYR:CE1	2.49	0.47
1:C:270:SER:HB3	1:C:323:GLN:NE2	2.30	0.47
1:C:307:LEU:HG	1:D:172:GLN:HE21	1.80	0.47
1:B:46:LYS:HD3	1:B:58:VAL:HB	1.97	0.46
1:B:5:VAL:HG22	1:B:92:ILE:CG2	2.46	0.46
1:D:103:LYS:O	1:D:107:GLU:HB3	2.15	0.46
1:C:122:ALA:HB1	1:C:123:PRO:HD2	1.98	0.46
1:A:299:VAL:HG12	1:A:308:VAL:HG22	1.97	0.46
1:D:57:THR:HG22	1:D:68:ASN:HA	1.97	0.46
1:A:4:LYS:HD3	1:A:89:GLY:O	2.15	0.46
1:D:119:VAL:HG13	1:D:147:ILE:CD1	2.46	0.46
1:D:256:VAL:HG23	1:D:299:VAL:HG22	1.98	0.46
1:C:66:GLU:OE2	1:C:69:GLY:CA	2.39	0.46
1:C:94:LEU:HD11	1:C:328:LEU:CD1	2.45	0.46
1:C:328:LEU:HD23	1:C:328:LEU:O	2.15	0.46
1:D:4:LYS:CE	1:D:30:THR:HG21	2.46	0.46
1:B:7:ILE:HD13	1:B:29:VAL:HG21	1.99	0.45
1:C:248:ALA:O	1:C:308:VAL:HG12	2.17	0.45
1:C:18:PHE:C	1:C:18:PHE:CD1	2.90	0.45
1:D:21:ILE:O	1:D:24:VAL:HG12	2.17	0.45
1:C:94:LEU:HD11	1:C:328:LEU:HD11	1.97	0.45
1:B:221:VAL:HG12	1:B:222:ILE:HG13	1.97	0.45
1:C:28:GLU:OE2	1:C:70:GLN:NE2	2.44	0.45
1:A:208:VAL:HG22	1:A:235:ARG:HB2	1.98	0.44
1:C:31:ARG:HD2	1:C:73:LYS:HD3	1.99	0.44
1:D:256:VAL:CG2	1:D:299:VAL:HG22	2.47	0.44
1:C:5:VAL:HG22	1:C:92:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLN:O	1:A:327:THR:HG23	2.17	0.44
1:C:103:LYS:HD2	1:C:146:VAL:HG21	1.99	0.44
1:C:129:LYS:HD3	1:C:139:ILE:HG22	1.98	0.44
1:B:225:LEU:HA	1:B:228:LYS:HD2	2.00	0.44
1:C:85:TRP:HE3	1:C:90:VAL:HG11	1.83	0.44
1:B:4:LYS:HD3	1:B:88:ASP:O	2.18	0.44
1:B:92:ILE:HD11	1:B:119:VAL:HG23	1.99	0.44
1:C:280:SER:HB3	1:D:207:ILE:HB	2.00	0.44
1:D:73:LYS:HE3	1:D:88:ASP:OD1	2.18	0.44
1:C:164:LEU:HD22	1:C:250:LEU:HD21	2.00	0.43
1:C:3:VAL:HG21	1:C:332:ALA:HB1	2.00	0.43
1:C:307:LEU:HG	1:D:172:GLN:NE2	2.33	0.43
1:A:94:LEU:HD23	1:A:119:VAL:HB	2.00	0.43
1:B:24:VAL:HG12	1:B:27:VAL:HG12	2.01	0.43
1:B:301:THR:CG2	1:B:306:GLN:HE21	2.32	0.43
1:A:236:VAL:HG11	1:B:236:VAL:HG11	2.01	0.43
1:C:315:ASP:O	1:C:316:ASN:C	2.57	0.42
1:A:296:GLN:HB2	1:A:311:VAL:CG2	2.48	0.42
1:D:21:ILE:HA	1:D:24:VAL:HG12	2.00	0.42
1:A:300:GLN:HE21	1:A:307:LEU:CD1	2.26	0.42
1:B:301:THR:HG22	1:B:306:GLN:HG2	2.00	0.42
1:A:38:PRO:HG3	1:A:74:VAL:CG2	2.50	0.42
1:A:198:ARG:HH11	1:A:209:PRO:HD2	1.85	0.42
1:A:299:VAL:HG23	1:A:299:VAL:O	2.20	0.42
1:B:273:TYR:N	1:B:291:LEU:CD1	2.82	0.42
1:C:152:CYS:HB3	2:C:401:NAD:C4N	2.50	0.42
1:B:35:LEU:HD13	2:B:401:NAD:C4A	2.49	0.42
1:C:292:PHE:HE1	1:C:310:VAL:HB	1.84	0.42
1:D:323:GLN:O	1:D:327:THR:HG23	2.20	0.42
1:C:130:THR:HG22	1:C:150:ALA:HB2	2.02	0.42
1:D:133:PHE:HB2	1:D:327:THR:HG22	2.02	0.42
1:C:85:TRP:O	1:C:90:VAL:HG12	2.19	0.41
1:A:133:PHE:HD2	1:A:134:ASN:OD1	2.02	0.41
1:C:334:ILE:HG22	1:C:334:ILE:O	2.20	0.41
1:C:136:ASN:HB2	1:C:139:ILE:HD13	2.03	0.41
1:A:292:PHE:HE1	1:A:310:VAL:HB	1.86	0.41
1:B:85:TRP:HE3	1:B:90:VAL:HG21	1.86	0.41
1:B:255:THR:OG1	1:B:258:GLU:HG3	2.21	0.41
1:C:24:VAL:HG12	1:C:27:VAL:HG12	2.02	0.41
1:A:3:VAL:HG21	1:A:332:ALA:HB1	2.02	0.41
1:B:64:GLY:HA2	1:B:74:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:VAL:HG11	1:D:236:VAL:HG11	2.03	0.41
1:D:24:VAL:HG13	1:D:27:VAL:HG13	2.00	0.41
1:D:255:THR:O	1:D:259:VAL:HG23	2.21	0.40
1:A:334:ILE:O	1:A:335:ALA:C	2.59	0.40
1:B:3:VAL:HG21	1:B:332:ALA:HB1	2.02	0.40
1:C:289:SER:HB3	1:C:323:GLN:CG	2.51	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	332/356 (93%)	307 (92%)	24 (7%)	1 (0%)	41	73
1	B	332/356 (93%)	307 (92%)	25 (8%)	0	100	100
1	C	323/356 (91%)	298 (92%)	24 (7%)	1 (0%)	41	73
1	D	307/356 (86%)	280 (91%)	27 (9%)	0	100	100
All	All	1294/1424 (91%)	1192 (92%)	100 (8%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ALA
1	C	70	GLN

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	269/288 (93%)	268 (100%)	1 (0%)	91	96
1	B	269/288 (93%)	269 (100%)	0	100	100
1	C	267/288 (93%)	267 (100%)	0	100	100
1	D	255/288 (88%)	254 (100%)	1 (0%)	91	96
All	All	1060/1152 (92%)	1058 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	D	20	ARG

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	22	GLN
1	A	108	GLN
1	A	300	GLN
1	B	134	ASN
1	C	108	GLN
1	C	113	ASN
1	C	126	ASN
1	C	210	ASN
1	D	172	GLN
1	D	323	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	NAD	B	401	-	42,48,48	0.64	0	50,73,73	0.74	1 (2%)
2	NAD	A	401	-	42,48,48	0.61	0	50,73,73	0.75	2 (4%)
2	NAD	C	401	-	42,48,48	0.61	0	50,73,73	0.74	1 (2%)
2	NAD	D	401	-	42,48,48	0.61	0	50,73,73	0.88	2 (4%)

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	B	401	-	-	6/26/62/62	0/5/5/5
2	NAD	A	401	-	-	8/26/62/62	0/5/5/5
2	NAD	C	401	-	-	8/26/62/62	0/5/5/5
2	NAD	D	401	-	-	9/26/62/62	0/5/5/5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAD	C6N-N1N-C2N	-3.03	119.21	121.97
2	B	401	NAD	C5A-C6A-N6A	2.44	124.06	120.35
2	C	401	NAD	C5A-C6A-N6A	2.37	123.95	120.35
2	A	401	NAD	C6N-N1N-C2N	-2.28	119.90	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAD	C5A-C6A-N6A	2.18	123.67	120.35
2	D	401	NAD	C5A-C6A-N6A	2.10	123.54	120.35

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C5B-O5B-PA-O1A
2	B	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	C5B-O5B-PA-O1A
2	C	401	NAD	C5B-O5B-PA-O2A
2	C	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	C5B-O5B-PA-O1A
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	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	C5B-O5B-PA-O3
2	B	401	NAD	C5B-O5B-PA-O3
2	C	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	C5B-O5B-PA-O2A
2	B	401	NAD	C5B-O5B-PA-O2A
2	C	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5B-O5B-PA-O2A
2	A	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	C2D-C1D-N1N-C6N

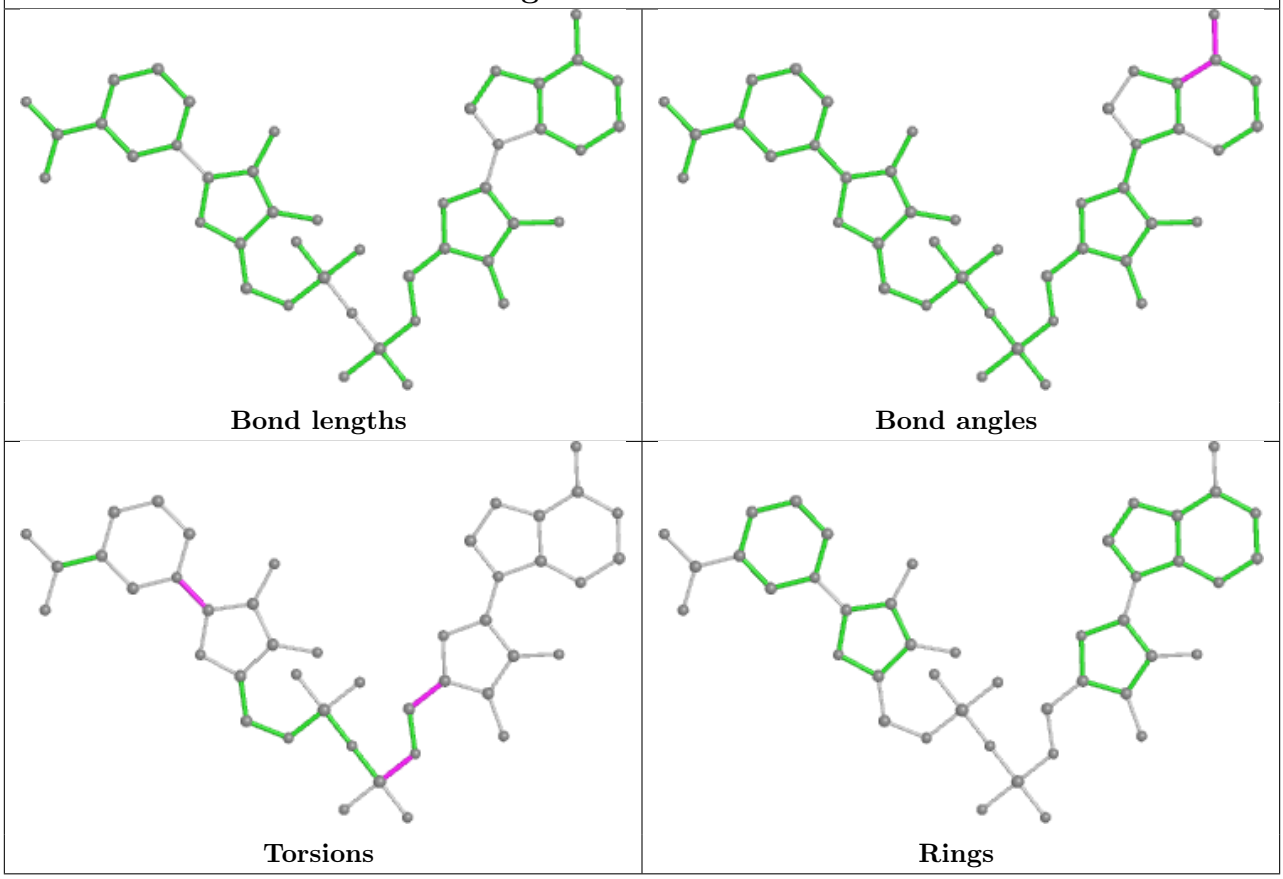
There are no ring outliers.

3 monomers are involved in 7 short contacts:

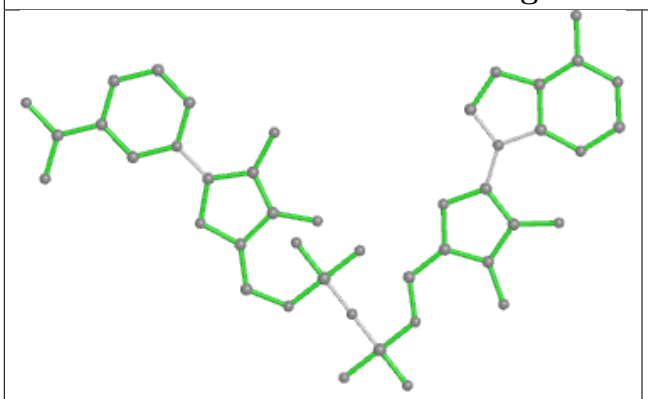
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	2	0
2	C	401	NAD	4	0
2	D	401	NAD	1	0

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

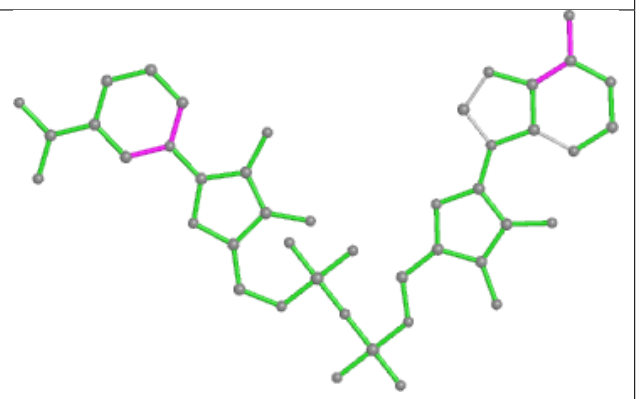
Ligand NAD B 401



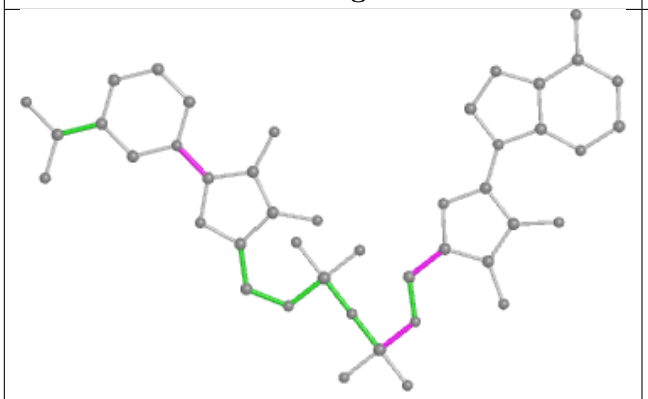
Ligand NAD A 401



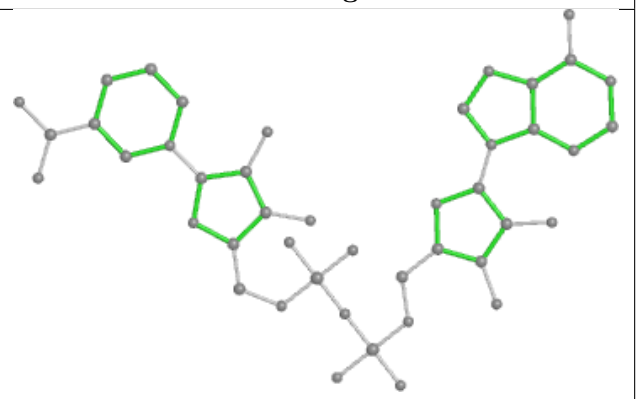
Bond lengths



Bond angles

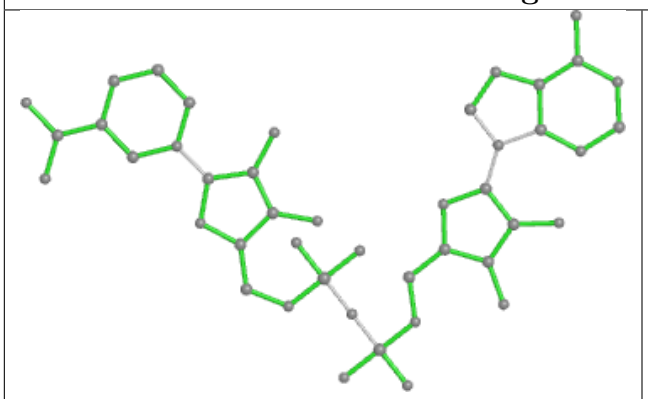


Torsions

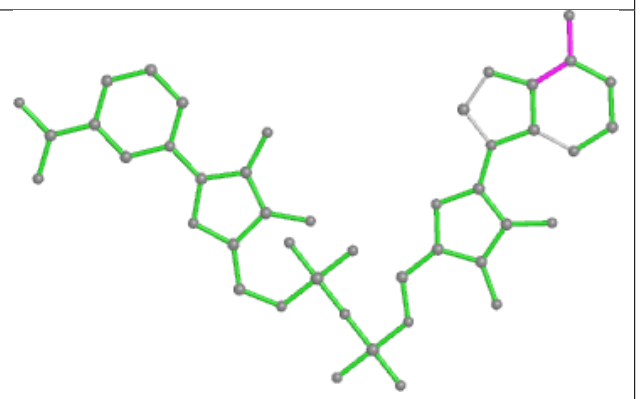


Rings

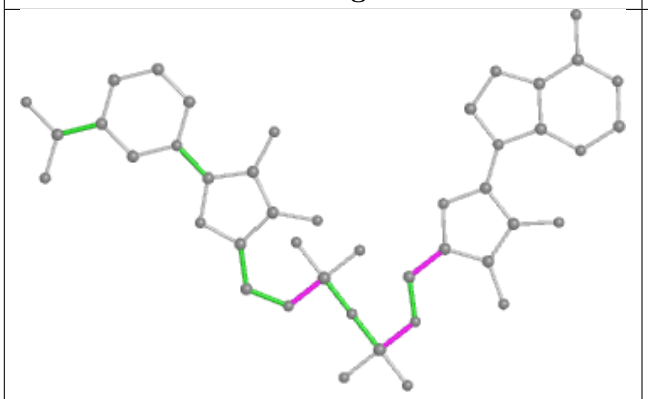
Ligand NAD C 401



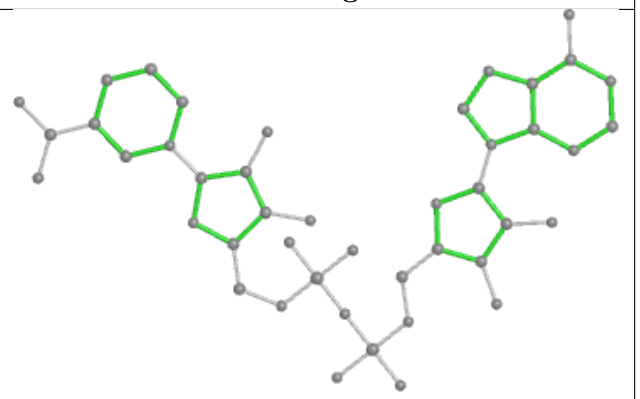
Bond lengths



Bond angles

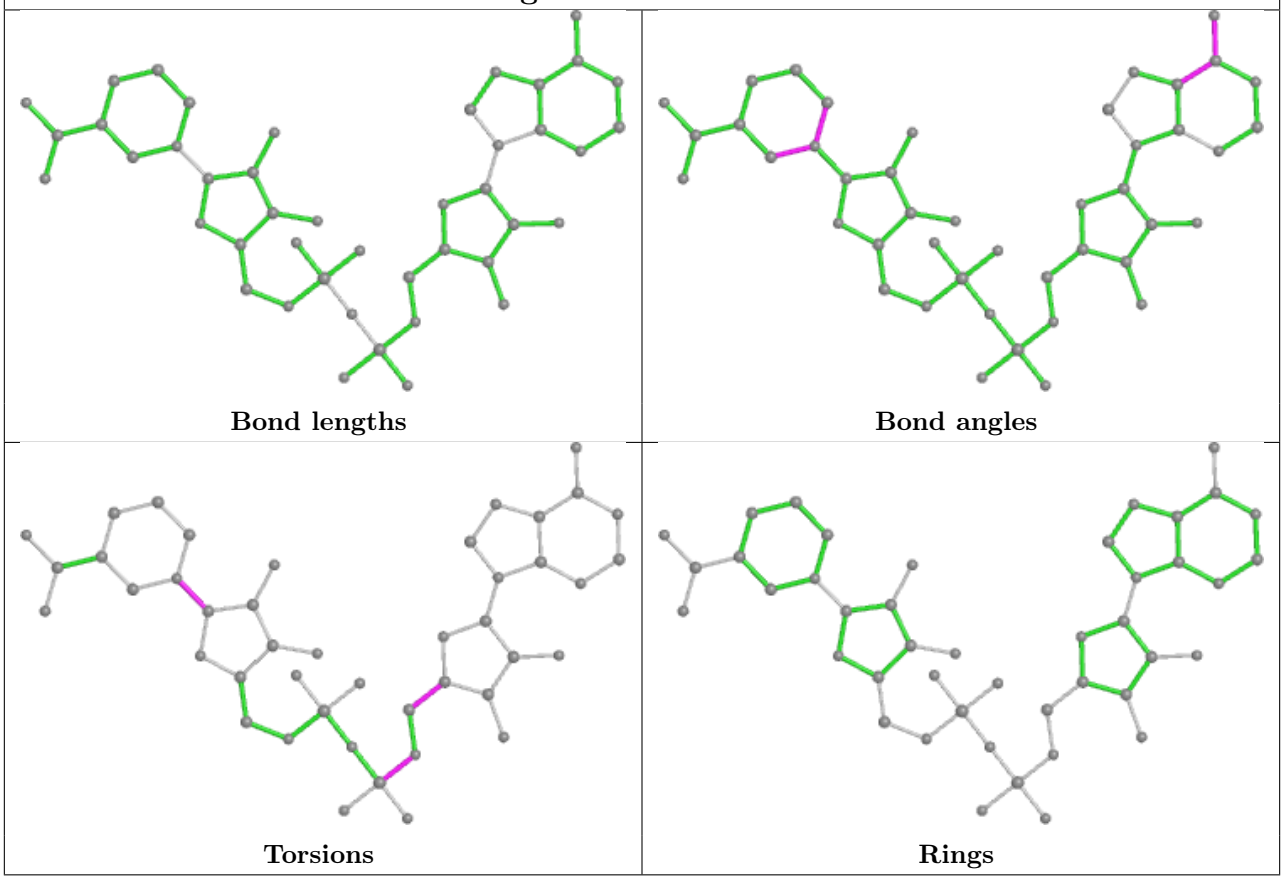


Torsions



Rings

Ligand NAD D 401



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	334/356 (93%)	0.04	0	100	100	45, 74, 98, 108	0
1	B	334/356 (93%)	-0.02	0	100	100	42, 72, 97, 118	0
1	C	329/356 (92%)	0.41	16 (4%)	29	18	53, 95, 123, 136	0
1	D	319/356 (89%)	0.53	24 (7%)	14	8	51, 101, 127, 150	0
All	All	1316/1424 (92%)	0.24	40 (3%)	50	34	42, 82, 119, 150	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	VAL	5.0
1	D	118	VAL	4.8
1	C	118	VAL	3.8
1	C	112	GLU	3.7
1	D	168	PHE	3.5
1	D	147	ILE	3.3
1	D	4	LYS	3.3
1	C	308	VAL	3.3
1	C	248	ALA	3.2
1	D	6	GLY	3.2
1	D	330	TYR	3.1
1	D	248	ALA	3.0
1	D	5	VAL	3.0
1	D	331	PHE	2.9
1	D	74	VAL	2.8
1	D	305	ASN	2.8
1	C	316	ASN	2.7
1	D	256	VAL	2.6
1	C	70	GLN	2.6
1	C	135	THR	2.6
1	C	330	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	2.4
1	D	94	LEU	2.4
1	C	120	ILE	2.3
1	C	250	LEU	2.3
1	D	126	ASN	2.3
1	C	140	LEU	2.3
1	D	29	VAL	2.2
1	D	100	PHE	2.2
1	C	119	VAL	2.2
1	D	91	GLU	2.2
1	D	164	LEU	2.1
1	D	255	THR	2.1
1	D	35	LEU	2.1
1	C	30	THR	2.1
1	C	138	ASP	2.1
1	D	9	GLY	2.1
1	C	332	ALA	2.0
1	C	231	GLY	2.0
1	D	260	ASN	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	MG	C	402	1/1	0.82	0.10	99,99,99,99	0
2	NAD	D	401	44/44	0.94	0.15	68,78,91,93	0
2	NAD	C	401	44/44	0.94	0.16	67,82,94,96	0
3	MG	A	402	1/1	0.95	0.07	65,65,65,65	0

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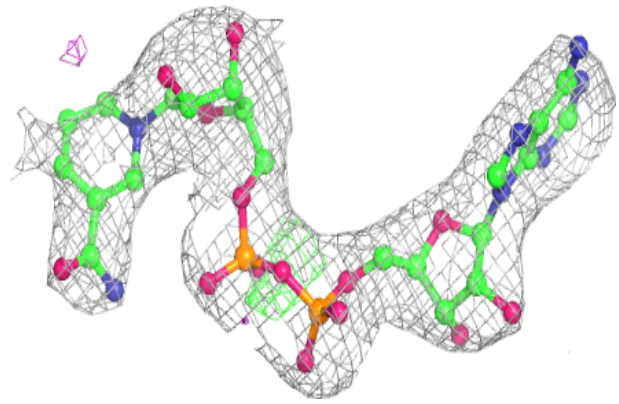
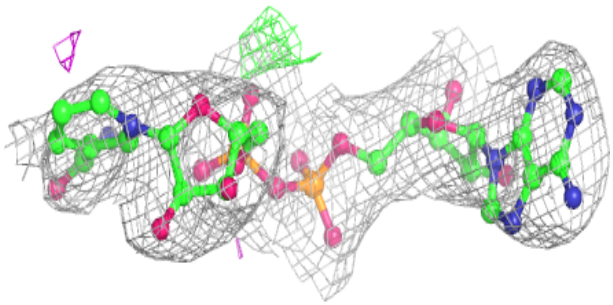
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	401	44/44	0.95	0.16	53,65,71,72	0
3	MG	D	402	1/1	0.95	0.08	80,80,80,80	0
2	NAD	B	401	44/44	0.97	0.14	46,58,66,68	0
3	MG	B	402	1/1	0.97	0.06	65,65,65,65	0

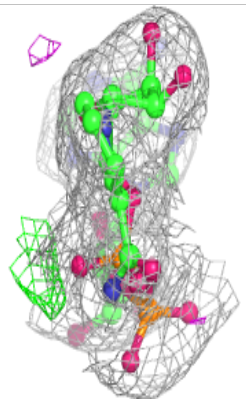
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

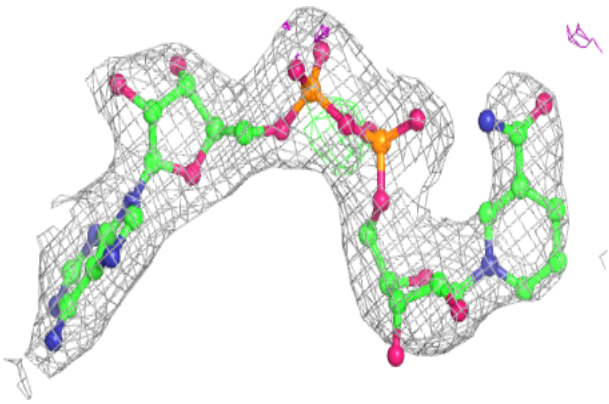


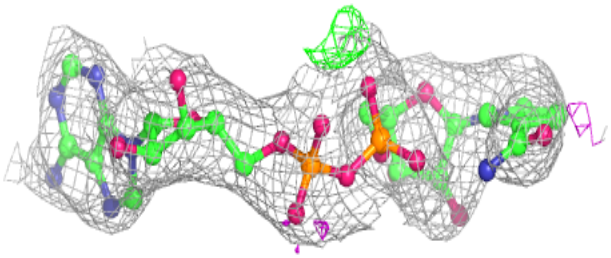


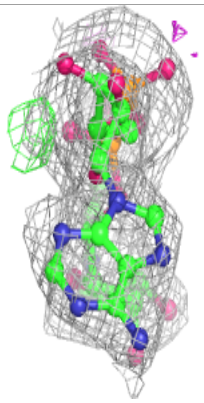


Electron density around NAD C 401:

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

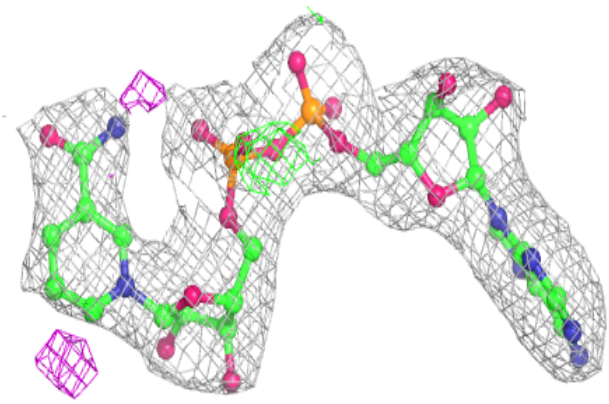


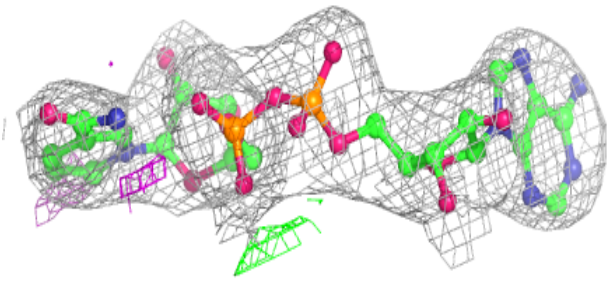


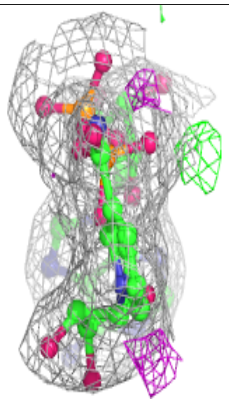


Electron density around NAD A 401:

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

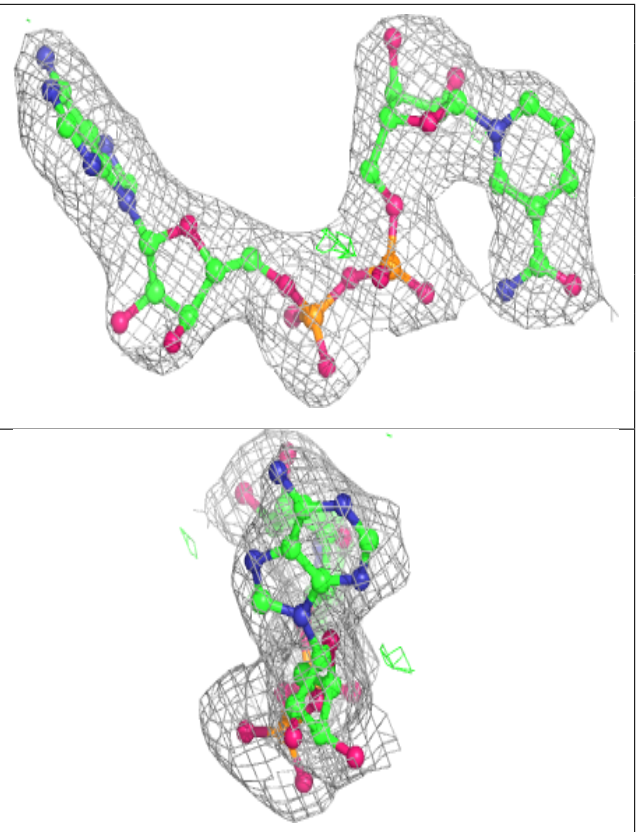






Electron density around NAD B 401:

$2mF_o$-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.