wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 03:36 am BST

PDB ID	:	1YBA
Title	:	The active form of phosphoglycerate dehydrogenase
Authors	:	Thompson, J.R.; Banaszak, L.J.
Deposited on	:	2004-12-20
Resolution	:	2.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

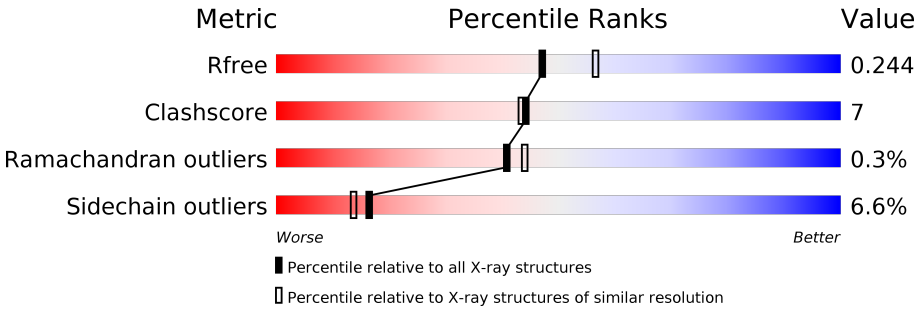
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)

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%

Mol	Chain	Length	Quality of chain
1	A	410	86% 12% ••
1	B	410	84% 14% ••
1	C	410	84% 13% ••
1	D	410	84% 12% ••

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
3	AKG	B	412	-	-	X	-
4	UNL	C	414	-	-	X	-
4	UNL	D	414	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14017 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 D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	Se	0	1	0
			3083	1950	535	586	4	8			
1	B	406	Total	C	N	O	S	Se	0	1	0
			3086	1952	535	587	4	8			
1	C	406	Total	C	N	O	S	Se	0	2	0
			3097	1958	540	587	4	8			
1	D	406	Total	C	N	O	S	Se	0	2	0
			3094	1956	536	590	4	8			

There are 32 discrepancies between the modelled and reference sequences:

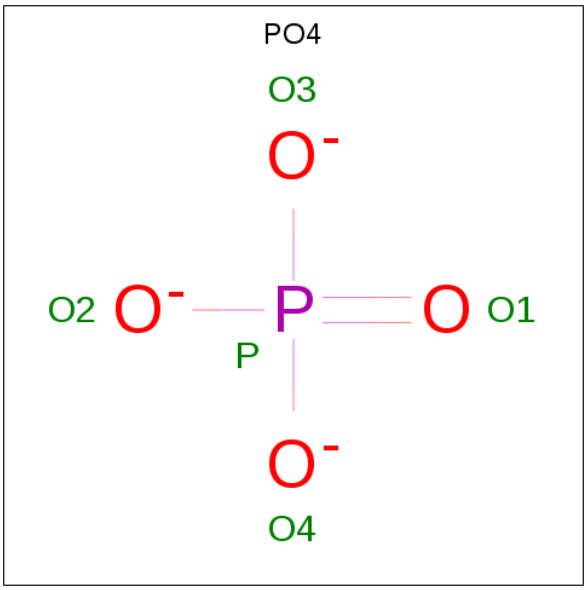
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	229	MSE	MET	MODIFIED RESIDUE	UNP P08328

Continued on next page...

Continued from previous page...

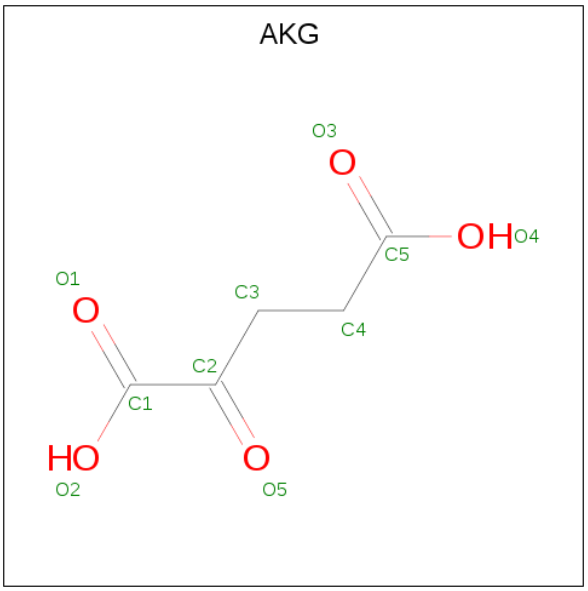
Chain	Residue	Modelled	Actual	Comment	Reference
C	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	397	MSE	MET	MODIFIED RESIDUE	UNP P08328

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).

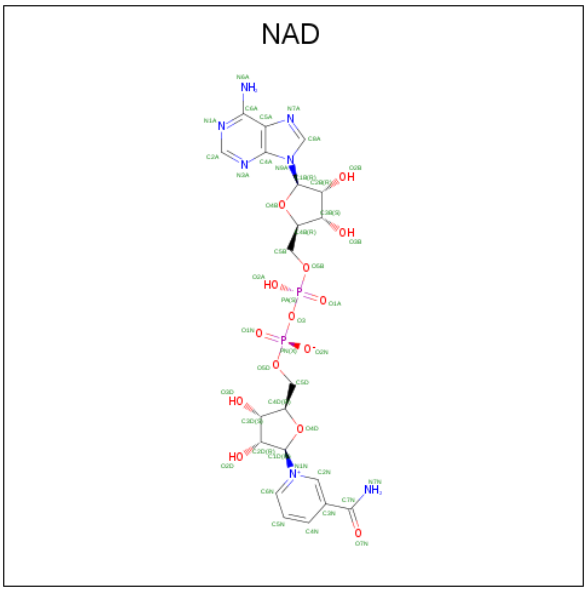


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 10 5 5	0	0
4	A	2	Total C O 20 10 10	0	0
4	D	2	Total C O 20 10 10	0	0
4	C	2	Total C O 20 10 10	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 6 is water.

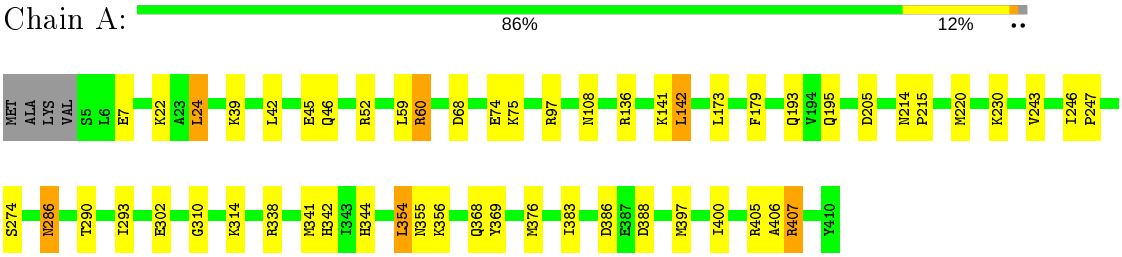
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		
6	B	330	Total	O	0	0
			330	330		
6	C	350	Total	O	0	0
			350	350		
6	D	366	Total	O	0	0
			366	366		

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. 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. 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.

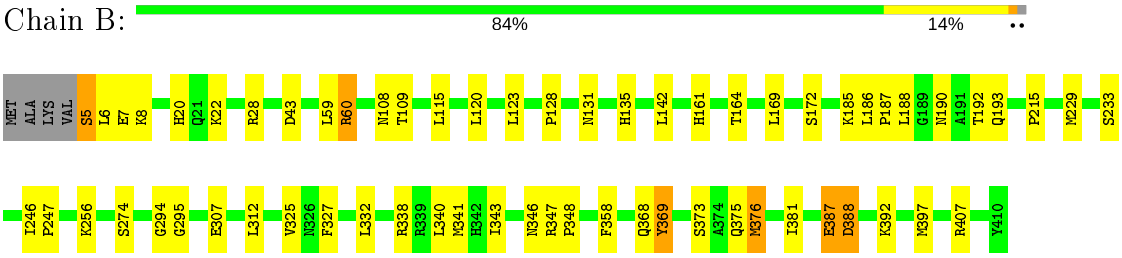
- Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain A:



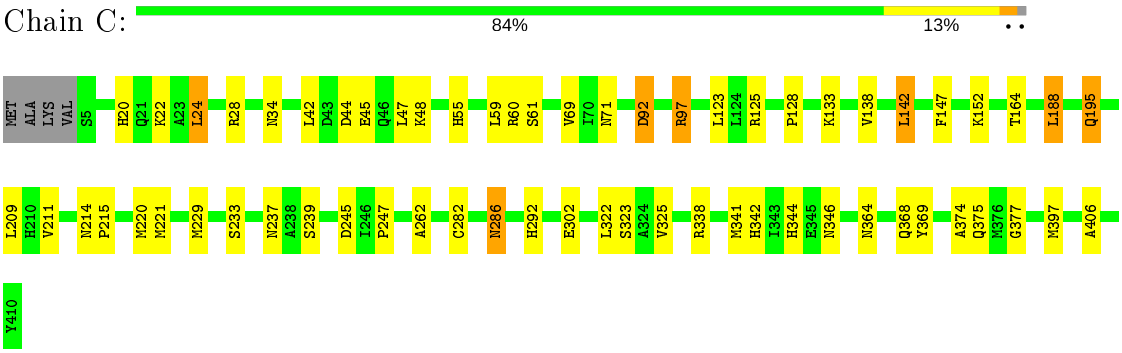
- Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain B:



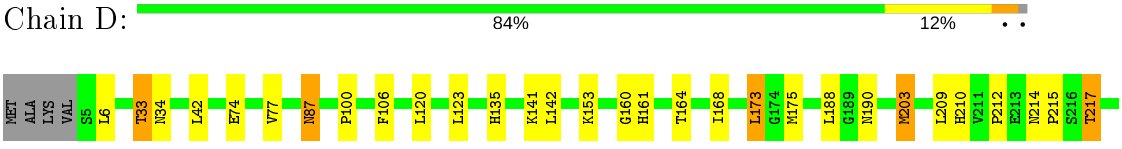
- Molecule 1: D-3-phosphoglycerate dehydrogenase

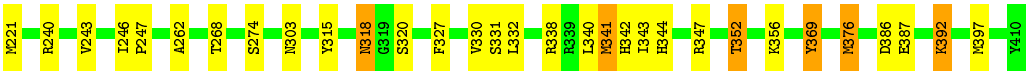
Chain C:



- Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain D:




M221
R240
V243
I246
P247
A262
T268
S274
N303
Y315
N318
G319
S320
F327
V330
S331
L332
R338
R339
L340
M341
H342
I343
H344
R347
T352
K356
Y369
M376
D386
E387
K392
M397
Y410

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	76.16Å 76.16Å 354.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 49.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.24) 94.2 (49.00-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	32.92 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.235 0.204 , 0.244	Depositor DCC
R_{free} test set	4538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14017	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: AKG, PO4, UNL, 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	0.74	0/3128	0.81	2/4224 (0.0%)
1	B	0.78	0/3131	0.81	4/4228 (0.1%)
1	C	0.75	0/3141	0.79	2/4239 (0.0%)
1	D	0.77	1/3139 (0.0%)	0.79	0/4239
All	All	0.76	1/12539 (0.0%)	0.80	8/16930 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	MSE	SE-CE	6.56	2.34	1.95

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	60	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	60	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	28	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	322	LEU	CB-CG-CD1	-5.33	101.94	111.00

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	3083	0	3120	34	0
1	B	3086	0	3121	36	0
1	C	3097	0	3135	57	0
1	D	3094	0	3124	42	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	4	0
3	C	10	0	4	2	0
3	D	10	0	4	0	0
4	A	20	0	0	0	0
4	B	10	0	0	1	0
4	C	20	0	0	2	0
4	D	20	0	0	2	0
5	A	44	0	26	0	0
5	B	44	0	26	1	0
5	C	44	0	26	0	0
5	D	44	0	26	0	0
6	A	300	0	0	5	0
6	B	330	0	0	6	0
6	C	350	0	0	7	0
6	D	366	0	0	7	0
All	All	14017	0	12620	168	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 7.

The worst 5 of 168 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:D:175:MSE:SE	1:D:175:MSE:CE	2.16	1.42
1:A:376:MSE:SE	1:A:376:MSE:CE	2.18	1.41
1:D:376:MSE:SE	1:D:376:MSE:CE	2.21	1.38
1:D:203:MSE:CE	1:D:203:MSE:SE	2.34	1.25
1:D:212:PRO:O	1:D:217:THR:HG21	1.66	0.96

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	405/410 (99%)	386 (95%)	18 (4%)	1 (0%)	47	53
1	B	405/410 (99%)	389 (96%)	14 (4%)	2 (0%)	29	28
1	C	406/410 (99%)	393 (97%)	13 (3%)	0	100	100
1	D	406/410 (99%)	383 (94%)	21 (5%)	2 (0%)	29	28
All	All	1622/1640 (99%)	1551 (96%)	66 (4%)	5 (0%)	41	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	GLU
1	B	43	ASP
1	D	6	LEU
1	A	386	ASP
1	B	215	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	329/323 (102%)	307 (93%)	22 (7%)	16	13
1	B	329/323 (102%)	305 (93%)	24 (7%)	14	10
1	C	330/323 (102%)	313 (95%)	17 (5%)	23	22
1	D	330/323 (102%)	307 (93%)	23 (7%)	15	12
All	All	1318/1292 (102%)	1232 (94%)	86 (6%)	16	14

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	369	TYR
1	C	42	LEU
1	D	347	ARG
1	B	375	GLN
1	B	387	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	368	GLN
1	C	108	ASN
1	D	318	ASN
1	B	395	GLN
1	C	34	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 7 are unknown - leaving 13 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	AKG	C	412	-	3,9,9	1.73	1 (33%)	4,11,11	2.27	2 (50%)
3	AKG	B	412	-	3,9,9	1.53	1 (33%)	4,11,11	1.38	1 (25%)
5	NAD	D	415	-	42,48,48	1.72	3 (7%)	50,73,73	1.67	10 (20%)
2	PO4	A	411	-	4,4,4	1.62	1 (25%)	6,6,6	1.08	0
2	PO4	C	411	-	4,4,4	1.02	0	6,6,6	1.06	0
2	PO4	B	411	-	4,4,4	0.95	0	6,6,6	2.36	2 (33%)
5	NAD	C	415	-	42,48,48	1.92	4 (9%)	50,73,73	1.54	7 (14%)
3	AKG	A	413	-	3,9,9	0.26	0	4,11,11	1.89	1 (25%)
5	NAD	A	416	-	42,48,48	2.02	5 (11%)	50,73,73	1.36	6 (12%)
5	NAD	B	414	-	42,48,48	1.75	5 (11%)	50,73,73	1.39	7 (14%)
3	AKG	D	412	-	3,9,9	1.84	2 (66%)	4,11,11	1.39	1 (25%)
2	PO4	D	411	-	4,4,4	1.22	1 (25%)	6,6,6	1.97	2 (33%)
2	PO4	A	412	-	4,4,4	0.71	0	6,6,6	0.45	0

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	AKG	C	412	-	-	0/3/9/9	-
5	NAD	B	414	-	-	7/26/62/62	0/5/5/5
5	NAD	D	415	-	-	6/26/62/62	0/5/5/5
5	NAD	C	415	-	-	5/26/62/62	0/5/5/5
3	AKG	A	413	-	-	3/3/9/9	-
5	NAD	A	416	-	-	6/26/62/62	0/5/5/5
3	AKG	B	412	-	-	3/3/9/9	-
3	AKG	D	412	-	-	1/3/9/9	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	416	NAD	O7N-C7N	9.63	1.42	1.24
5	D	415	NAD	O7N-C7N	9.27	1.41	1.24
5	C	415	NAD	O7N-C7N	9.08	1.41	1.24
5	B	414	NAD	O7N-C7N	8.12	1.39	1.24
5	A	416	NAD	C2A-N3A	5.37	1.40	1.32

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	415	NAD	O4D-C1D-C2D	-5.69	98.62	106.93
5	D	415	NAD	N3A-C2A-N1A	-5.38	120.26	128.68
5	A	416	NAD	C4A-C5A-N7A	-4.77	104.43	109.40
5	C	415	NAD	N3A-C2A-N1A	-4.64	121.43	128.68
5	C	415	NAD	O7N-C7N-C3N	-4.63	114.09	119.63

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	412	AKG	C2-C3-C4-C5
5	D	415	NAD	O4D-C1D-N1N-C6N
5	A	416	NAD	O4D-C1D-N1N-C2N
5	A	416	NAD	O4D-C1D-N1N-C6N
5	A	416	NAD	C2D-C1D-N1N-C2N

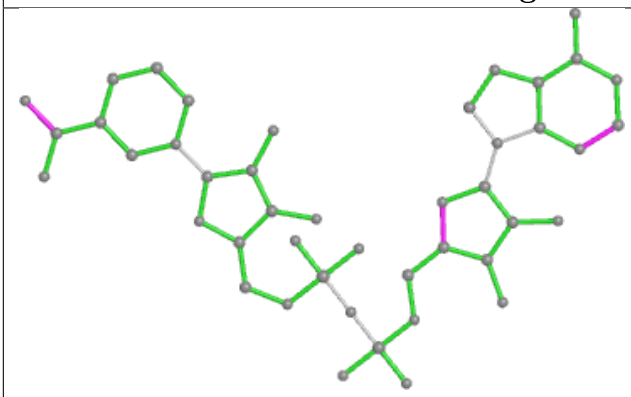
There are no ring outliers.

3 monomers are involved in 7 short contacts:

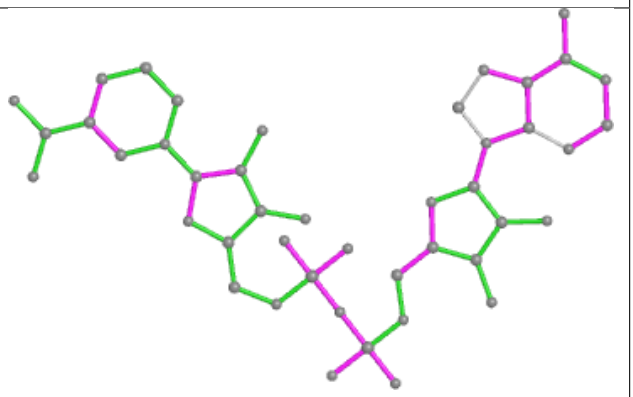
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	412	AKG	2	0
3	B	412	AKG	4	0
5	B	414	NAD	1	0

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.

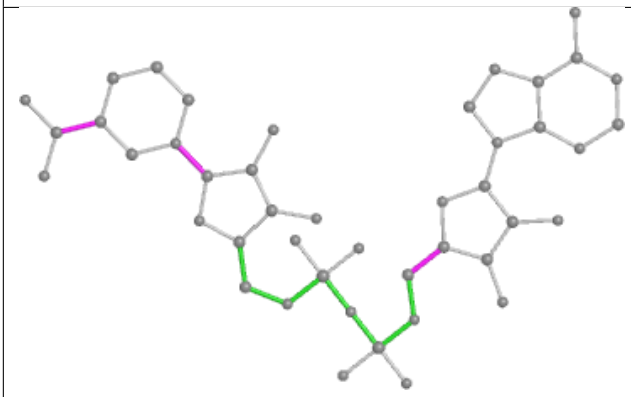
Ligand NAD D 415



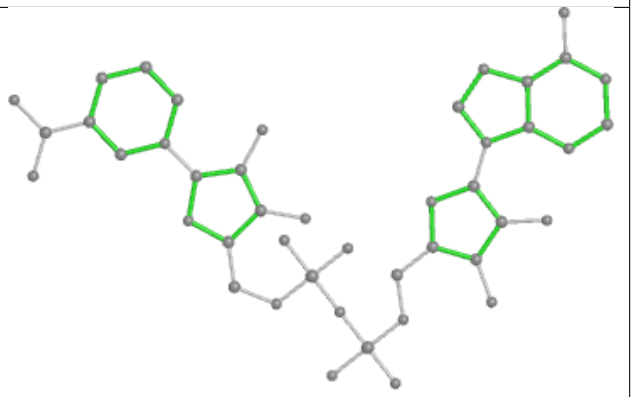
Bond lengths



Bond angles

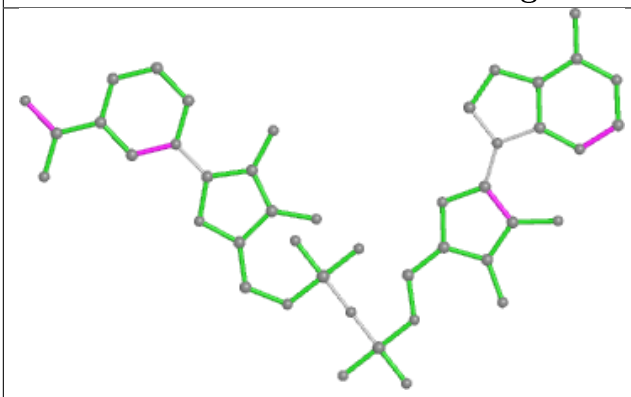


Torsions

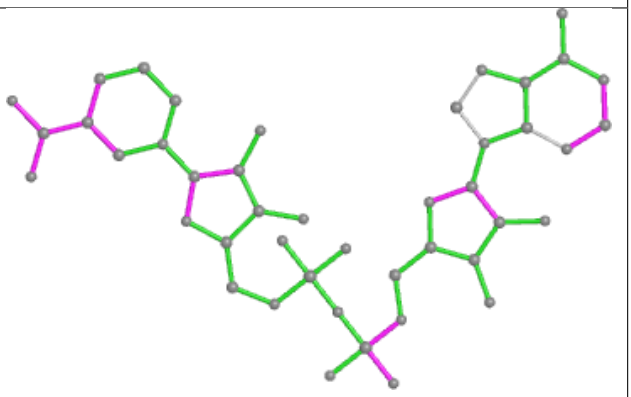


Rings

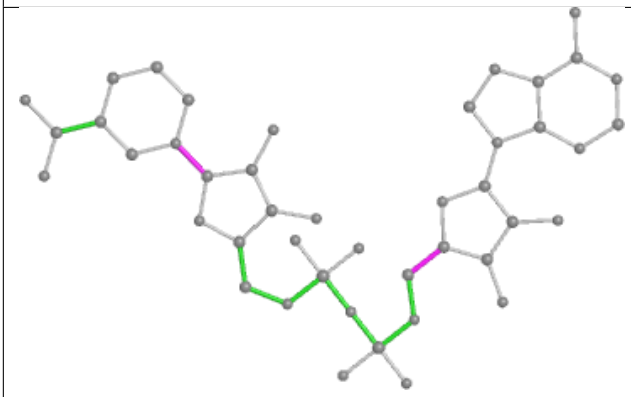
Ligand NAD C 415



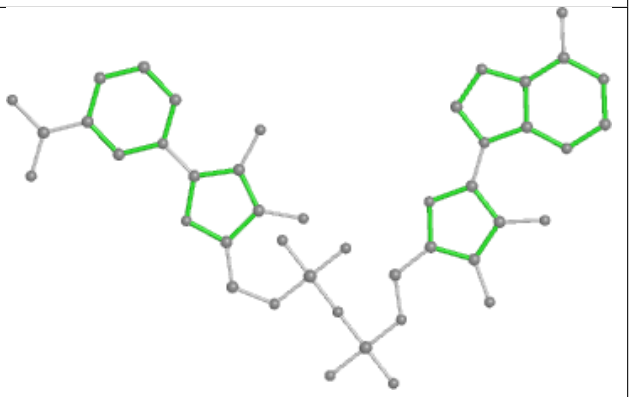
Bond lengths



Bond angles

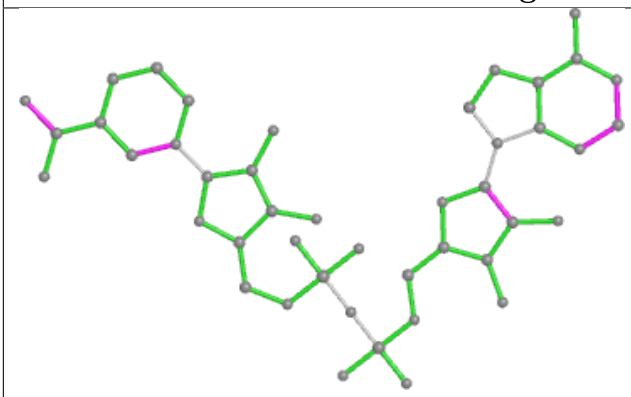


Torsions

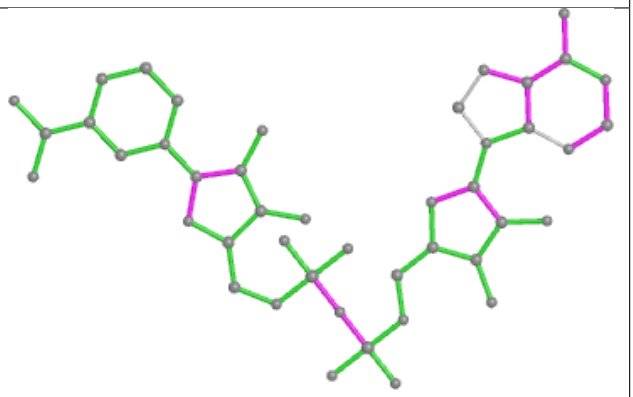


Rings

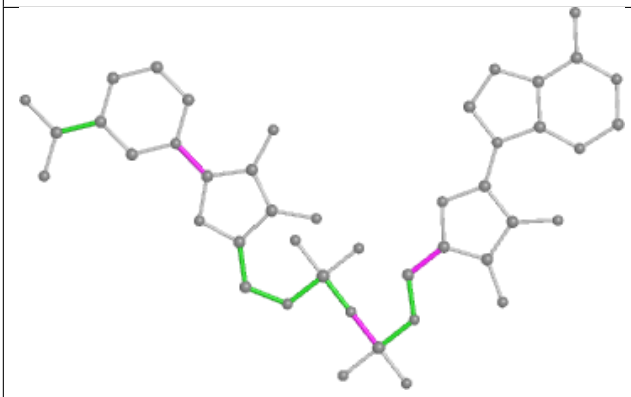
Ligand NAD A 416



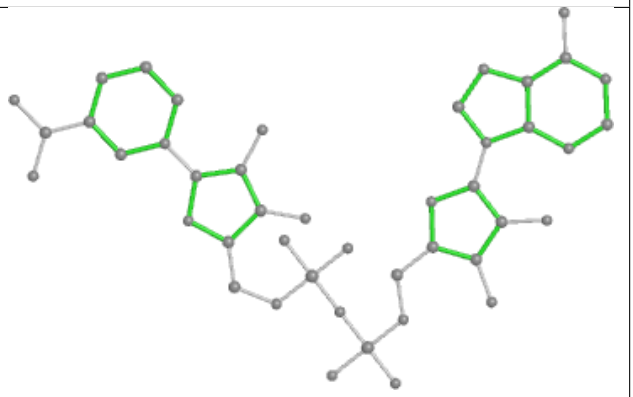
Bond lengths



Bond angles

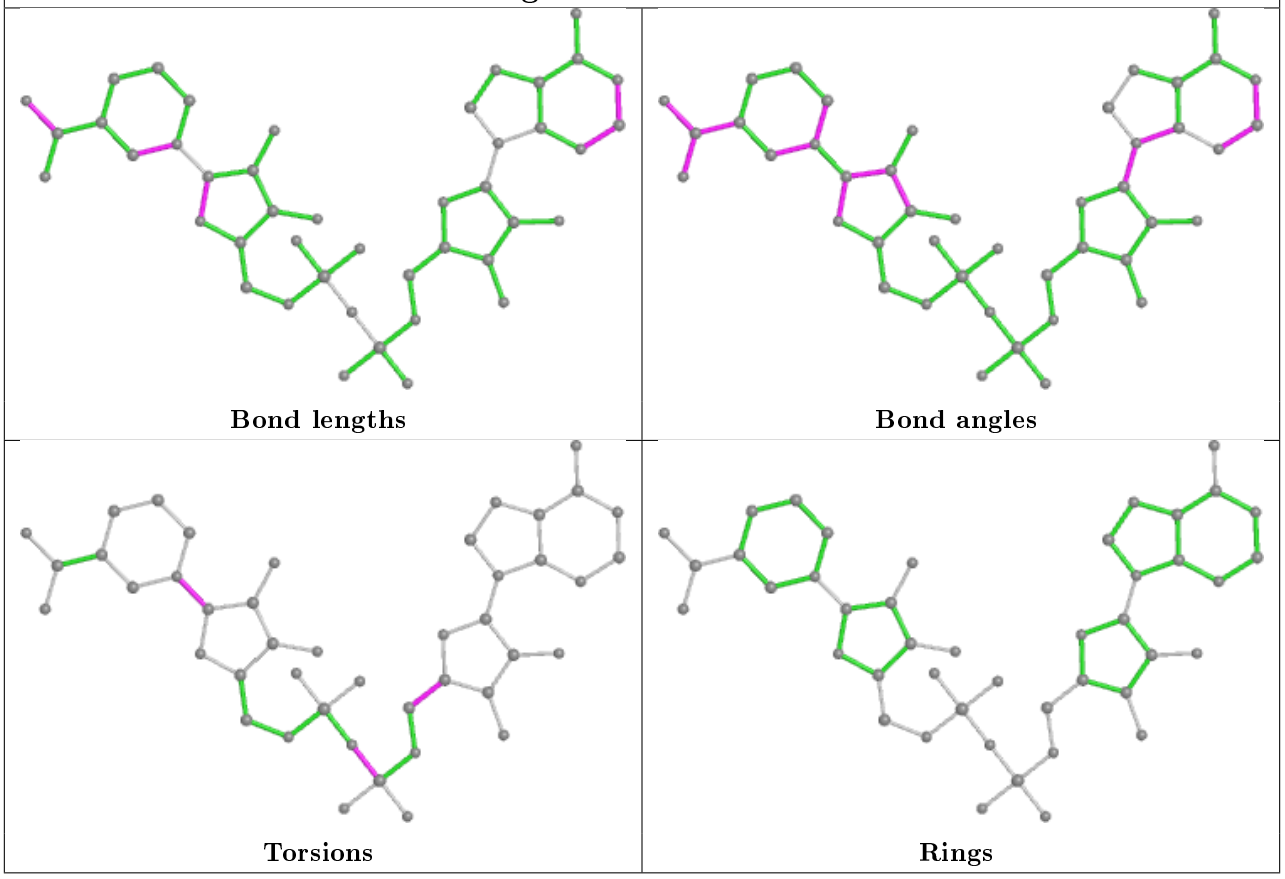


Torsions



Rings

Ligand NAD B 414



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

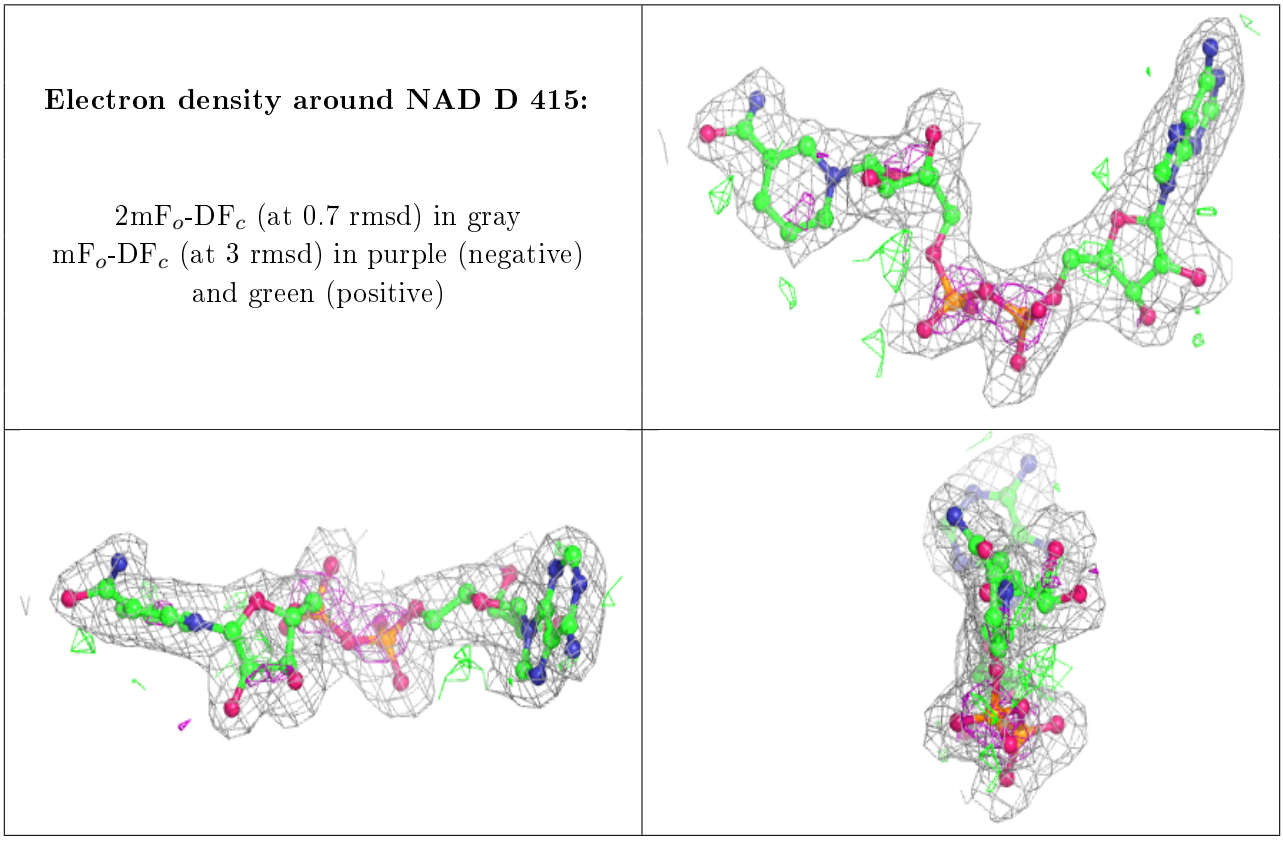
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

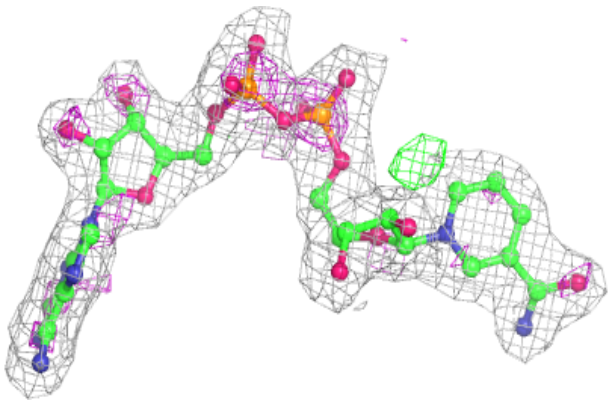
Electron density around NAD D 415:

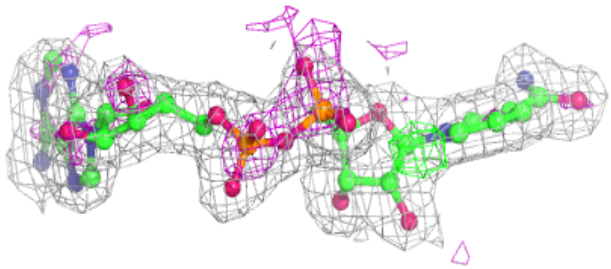
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

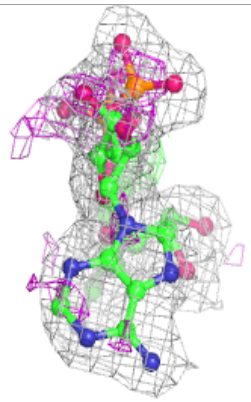


Electron density around NAD A 416:

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

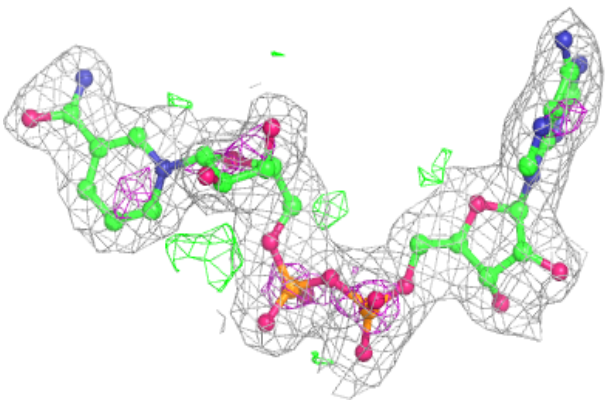


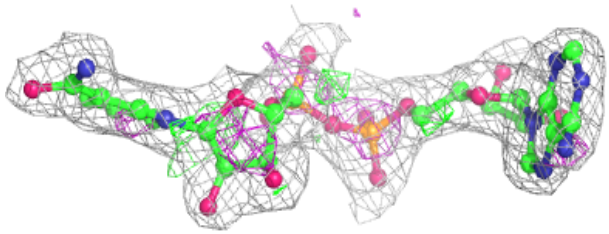


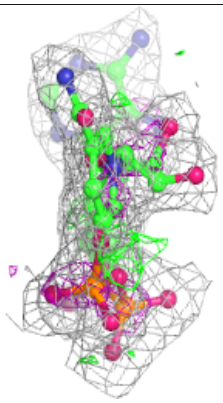


Electron density around NAD B 414:

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

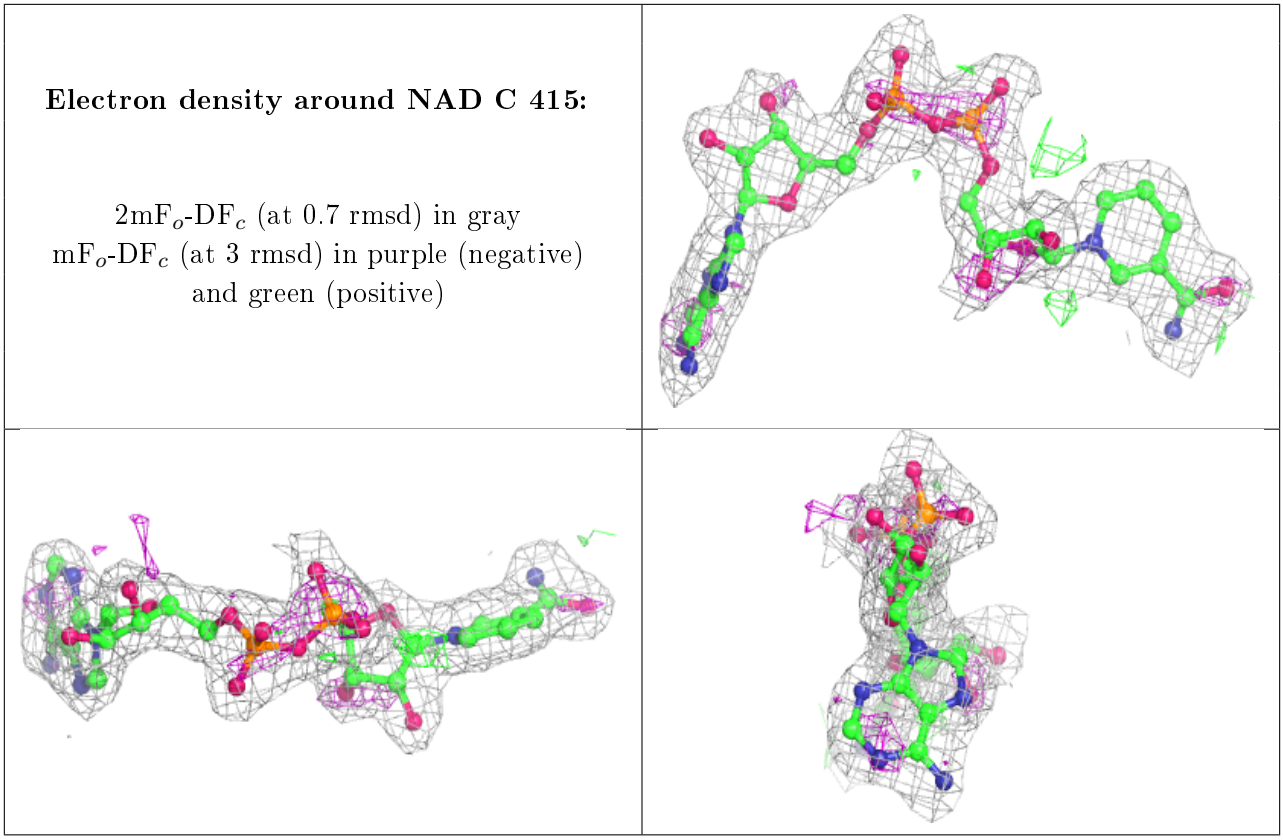






Electron density around NAD C 415:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.