Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 04:00 PM EDT

PDB ID	:	1NZX
Title	:	Human mitochondrial aldehyde dehydrogenase complexed with NAD+ in the presence of low Mg2+
Authors	:	Perez-Miller, S.J.; Hurley, T.D.
Deposited on	:	2003-02-20
Resolution	:	2.45 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:

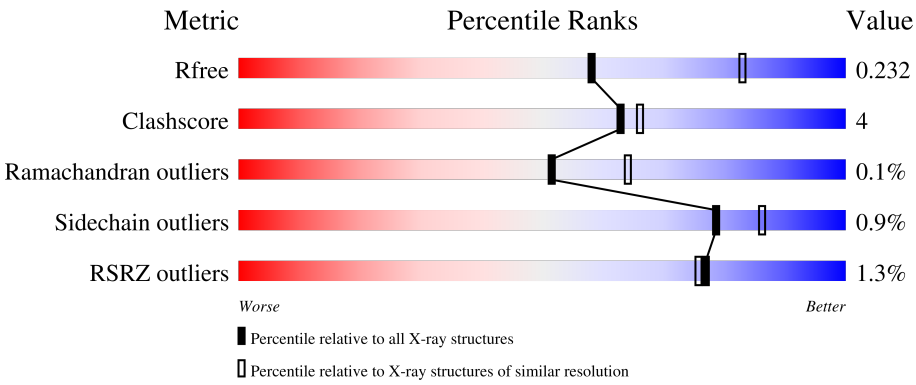
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	500	2% 88% 11% •
1	B	500	% 87% 12% •
1	C	500	91% 8% •
1	D	500	3% 86% 12% •
1	E	500	89% 10% •

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Mol	Chain	Length	Quality of chain
1	F	500	%, 88%, 11%
1	G	500	%, 89%, 9%
1	H	500	3%, 85%, 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	C	1703	-	-	-	X
2	NA	D	1704	-	-	-	X
2	NA	H	1708	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32014 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3798	2415	648	717	18	0	0	0
1	B	494	3798	2415	648	717	18	0	0	0
1	C	494	3798	2415	648	717	18	0	0	0
1	D	494	3798	2415	648	717	18	0	0	0
1	E	494	3798	2415	648	717	18	0	0	0
1	F	494	3798	2415	648	717	18	0	0	0
1	G	494	3798	2415	648	717	18	0	0	0
1	H	494	3798	2415	648	717	18	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

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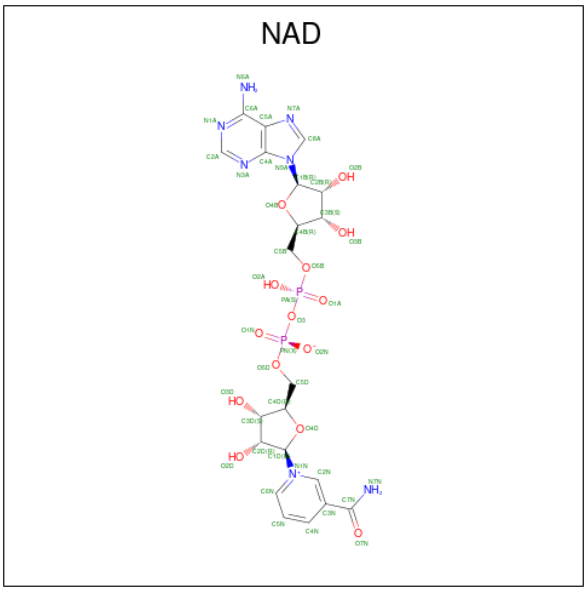
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	G	1	1	1	0	0
			Total	Na		
2	H	1	1	1	0	0

- 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
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	D	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	E	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	F	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	G	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	H	1	27	10	5	10	2	0	0

- Molecule 4 is water.

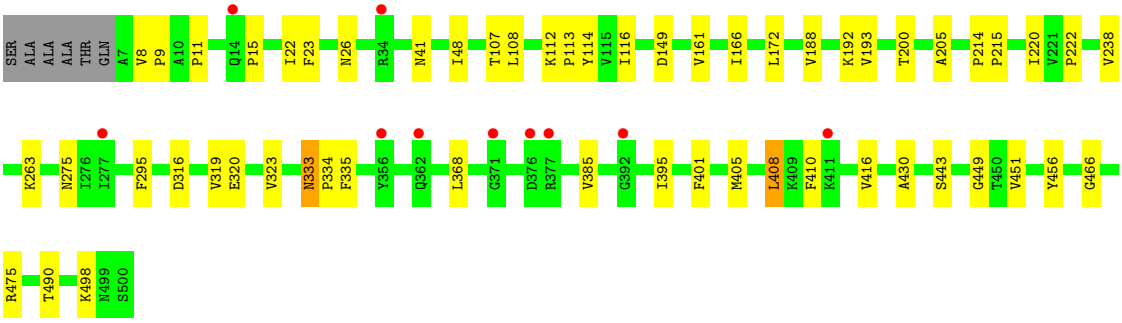
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	164	164	164	0	0
			Total	O		
4	B	177	177	177	0	0
			Total	O		
4	C	198	198	198	0	0
			Total	O		
4	D	118	118	118	0	0
			Total	O		
4	E	187	187	187	0	0
			Total	O		
4	F	239	239	239	0	0
			Total	O		
4	G	187	187	187	0	0
			Total	O		
4	H	136	136	136	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.

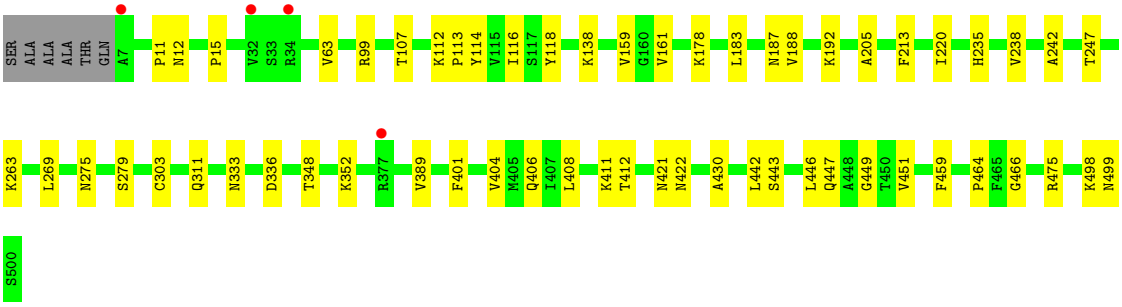
• Molecule 1: Aldehyde dehydrogenase

Chain A:



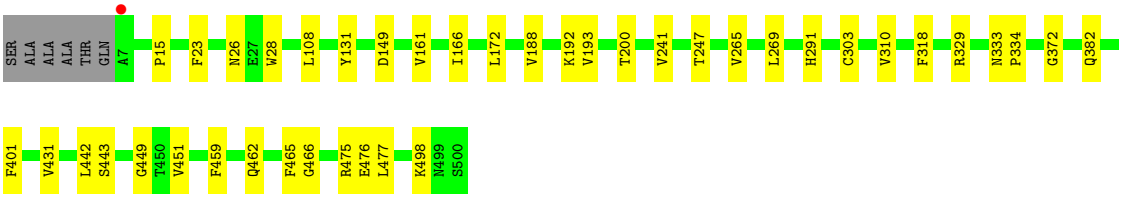
• Molecule 1: Aldehyde dehydrogenase

Chain B:



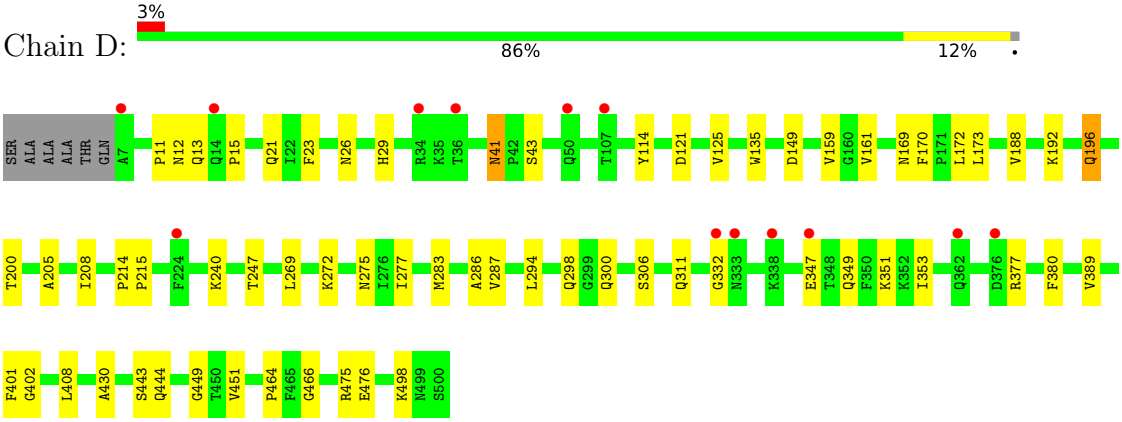
• Molecule 1: Aldehyde dehydrogenase

Chain C:



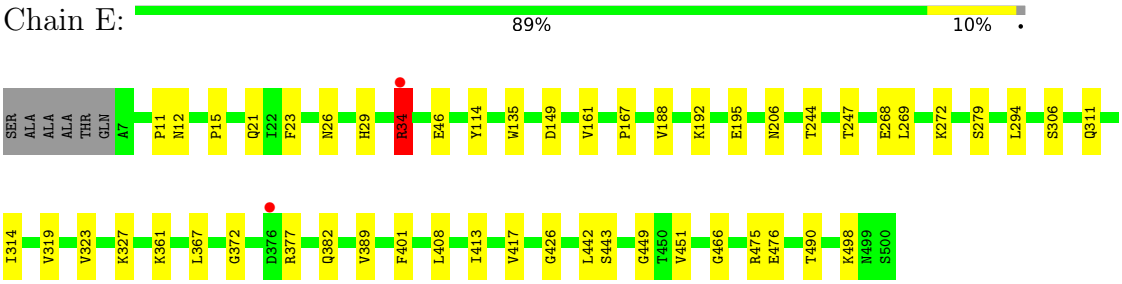
• Molecule 1: Aldehyde dehydrogenase

Chain D:



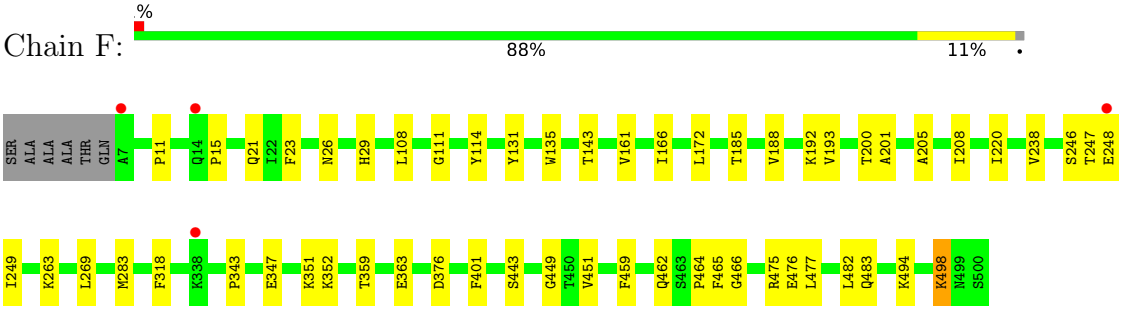
• Molecule 1: Aldehyde dehydrogenase

Chain E:



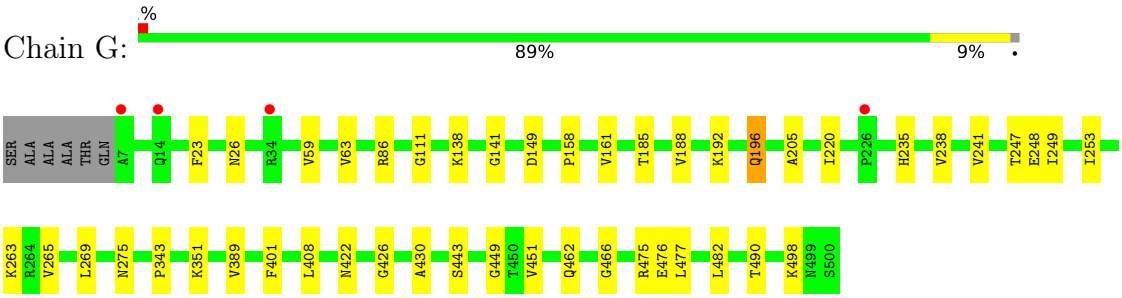
• Molecule 1: Aldehyde dehydrogenase

Chain F:



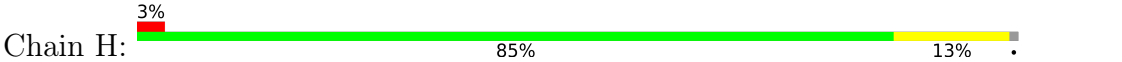
• Molecule 1: Aldehyde dehydrogenase

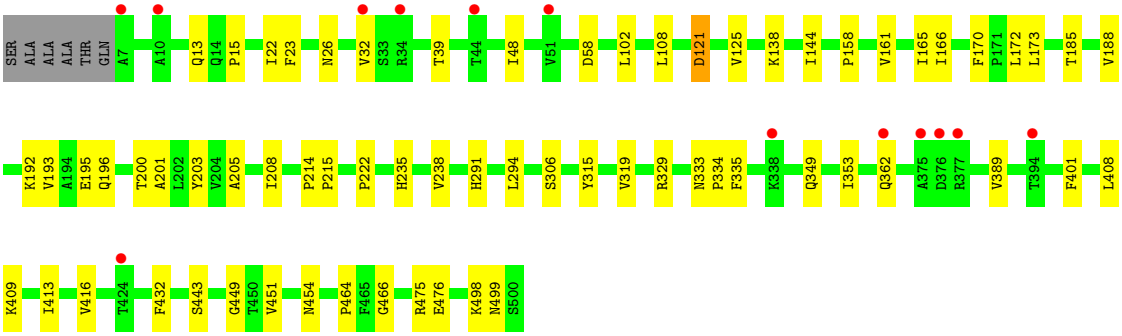
Chain G:



• Molecule 1: Aldehyde dehydrogenase

Chain H:




SER
ALA
ALA
ALA
THR
GLN
A7
A10
Q13
Q14
P15
I22
F23
N26
V32
S33
R34
T39
T44
I48
V51
D58
L102
L108
D121
V125
K138
I144
P158
V161
I165
I166
F170
P171
L172
L173
T185
V188
K192
V193
A194
E195
Q196
T200
A201
L202
Y203
V204
A205
I208
P214
P215
P222
H235
V238
H291
L294
S306
Y315
V319
R329
N333
P334
F335
K338
Q349
I353
Q362
A375
D376
R377
V389
T394
F401
L408
K409
I413
V416
T424
F432
S443
G449
T450
V451
N454
P464
F465
G466
R475
E476
K498
N499
S500

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.31Å 151.10Å 176.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.45 19.99 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.99-2.45) 96.6 (19.99-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.245 0.198 , 0.232	Depositor DCC
R_{free} test set	6757 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32014	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3490e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.38	0/3882	0.57	0/5267
1	B	0.37	0/3882	0.57	0/5267
1	C	0.37	0/3882	0.58	0/5267
1	D	0.37	0/3882	0.57	0/5267
1	E	0.38	0/3882	0.59	2/5267 (0.0%)
1	F	0.38	0/3882	0.58	0/5267
1	G	0.38	0/3882	0.58	0/5267
1	H	0.38	0/3882	0.57	0/5267
All	All	0.38	0/31056	0.58	2/42136 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	34	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	34	ARG	NE-CZ-NH1	6.31	123.45	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	3798	0	3745	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3798	0	3745	34	0
1	C	3798	0	3745	23	0
1	D	3798	0	3745	41	0
1	E	3798	0	3745	29	0
1	F	3798	0	3745	38	0
1	G	3798	0	3745	31	0
1	H	3798	0	3745	41	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	1	0
4	A	164	0	0	1	0
4	B	177	0	0	0	0
4	C	198	0	0	1	0
4	D	118	0	0	1	0
4	E	187	0	0	3	0
4	F	239	0	0	0	0
4	G	187	0	0	2	0
4	H	136	0	0	1	0
All	All	32014	0	30056	258	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 4.

All (258) 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:41:ASN:HB2	1:A:48:ILE:HD11	1.43	1.00
1:E:247:THR:HA	1:E:269:LEU:HD13	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:GLN:H	1:G:196:GLN:HE21	1.28	0.82
1:F:283:MET:HA	1:F:283:MET:HE2	1.67	0.77
1:D:196:GLN:H	1:D:196:GLN:HE21	1.35	0.74
1:A:333:ASN:ND2	1:A:335:PHE:H	1.87	0.73
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.74	0.69
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.74	0.69
1:D:247:THR:HA	1:D:269:LEU:HD13	1.78	0.66
1:D:277:ILE:HD12	1:D:286:ALA:HB1	1.79	0.64
1:A:333:ASN:HD22	1:A:335:PHE:H	1.45	0.63
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.30	0.62
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.82	0.62
1:C:166:ILE:HD11	1:C:193:VAL:HG12	1.82	0.62
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.82	0.62
1:E:361:LYS:HE2	1:E:367:LEU:HD22	1.82	0.62
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.81	0.62
1:C:172:LEU:HD21	1:C:200:THR:HB	1.82	0.61
1:D:41:ASN:ND2	1:D:43:SER:H	1.98	0.61
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.64	0.61
1:B:411:LYS:HG2	1:B:412:THR:HG23	1.82	0.60
1:D:349:GLN:O	1:D:353:ILE:HG13	2.02	0.60
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.36	0.60
1:H:315:TYR:CG	1:H:409:LYS:HE2	2.37	0.60
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.82	0.59
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.37	0.59
1:B:275:ASN:ND2	1:B:430:ALA:HB3	2.17	0.59
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.38	0.58
1:D:283:MET:O	1:D:287:VAL:HG23	2.04	0.57
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.86	0.57
1:F:247:THR:HA	1:F:269:LEU:HD13	1.86	0.57
1:D:353:ILE:HD13	1:D:402:GLY:HA3	1.85	0.57
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.39	0.57
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.28	0.57
1:F:185:THR:HG23	1:F:482:LEU:HD22	1.86	0.57
1:D:205:ALA:HA	1:D:208:ILE:HD12	1.87	0.56
1:A:107:THR:HG23	1:A:112:LYS:O	2.05	0.56
1:A:333:ASN:HD22	1:A:333:ASN:C	2.09	0.56
1:A:22:ILE:HG12	1:A:222:PRO:HD2	1.87	0.55
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.21	0.55
1:B:275:ASN:HD22	1:B:430:ALA:HB3	1.71	0.55
1:B:247:THR:HA	1:B:269:LEU:HD13	1.87	0.55
1:D:41:ASN:C	1:D:41:ASN:HD22	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:VAL:O	1:B:263:LYS:HE3	2.07	0.55
1:A:443:SER:HA	1:A:451:VAL:HG11	1.89	0.55
1:G:241:VAL:CG1	1:G:265:VAL:HG22	2.37	0.55
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.42	0.54
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.42	0.54
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.42	0.54
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.88	0.54
1:H:443:SER:HA	1:H:451:VAL:HG11	1.89	0.54
1:D:121:ASP:O	1:D:125:VAL:HG23	2.07	0.54
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.90	0.54
1:B:12:ASN:O	1:B:15:PRO:HD3	2.07	0.54
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.90	0.54
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.89	0.53
1:F:283:MET:HE2	1:F:283:MET:CA	2.37	0.53
1:F:131:TYR:CE1	1:F:462:GLN:HG3	2.44	0.53
1:D:161:VAL:HA	1:D:188:VAL:HG23	1.91	0.53
1:G:408:LEU:N	1:G:408:LEU:HD12	2.24	0.53
1:A:316:ASP:O	1:A:320:GLU:HG3	2.09	0.53
1:F:283:MET:HE1	1:F:318:PHE:HD1	1.74	0.52
1:H:195:GLU:HG2	1:H:196:GLN:OE1	2.09	0.52
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.92	0.52
1:C:15:PRO:HG2	1:C:108:LEU:HD22	1.92	0.52
1:A:161:VAL:HA	1:A:188:VAL:HG23	1.92	0.52
1:E:161:VAL:HA	1:E:188:VAL:HG23	1.92	0.52
1:H:161:VAL:HA	1:H:188:VAL:HG23	1.91	0.52
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.92	0.52
1:A:172:LEU:HD21	1:A:200:THR:HB	1.91	0.52
1:A:319:VAL:O	1:A:323:VAL:HG23	2.11	0.51
1:B:107:THR:HG23	1:B:112:LYS:O	2.11	0.51
1:C:291:HIS:HE1	1:C:329:ARG:HH11	1.59	0.51
1:F:11:PRO:HB3	1:F:114:TYR:CE2	2.45	0.51
1:F:205:ALA:HA	1:F:208:ILE:HD12	1.92	0.51
1:E:311:GLN:HG3	4:E:5667:HOH:O	2.10	0.51
1:E:319:VAL:O	1:E:323:VAL:HG23	2.10	0.51
1:G:241:VAL:HG12	1:G:265:VAL:HG22	1.94	0.50
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.47	0.50
1:G:149:ASP:HA	1:G:498:LYS:HB2	1.94	0.50
1:H:121:ASP:O	1:H:125:VAL:HG23	2.11	0.50
1:F:166:ILE:HD11	1:F:193:VAL:HG12	1.94	0.50
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.94	0.50
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:MET:HE1	1:F:318:PHE:CD1	2.48	0.49
1:B:63:VAL:HG21	1:B:235:HIS:CD2	2.47	0.49
1:F:248:GLU:HG3	1:F:249:ILE:N	2.28	0.49
1:C:247:THR:HA	1:C:269:LEU:HD13	1.93	0.49
1:D:11:PRO:HB3	1:D:114:TYR:CE1	2.47	0.49
1:B:498:LYS:HG2	1:B:499:ASN:N	2.28	0.49
1:G:389:VAL:HB	1:G:408:LEU:HG	1.94	0.49
1:A:333:ASN:HD22	1:A:334:PRO:N	2.11	0.48
1:B:11:PRO:HB3	1:B:114:TYR:CE1	2.48	0.48
1:F:172:LEU:HD21	1:F:200:THR:HB	1.95	0.48
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.48	0.48
1:G:63:VAL:HG11	1:G:235:HIS:CE1	2.48	0.48
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.14	0.48
1:F:246:SER:OG	1:F:248:GLU:HG2	2.13	0.48
1:D:347:GLU:CG	1:D:351:LYS:HE3	2.44	0.48
1:B:389:VAL:HB	1:B:408:LEU:HG	1.95	0.48
1:D:311:GLN:HG3	4:D:4569:HOH:O	2.13	0.48
1:H:362:GLN:OE1	1:H:362:GLN:HA	2.14	0.48
1:B:138:LYS:HE3	1:D:135:TRP:CD1	2.49	0.48
1:B:279:SER:HB3	1:B:311:GLN:OE1	2.14	0.47
4:E:5689:HOH:O	1:F:483:GLN:HB3	2.13	0.47
1:A:15:PRO:HG2	1:A:108:LEU:HD22	1.95	0.47
1:F:449:GLY:HA3	1:F:466:GLY:O	2.14	0.47
1:C:459:PHE:HE2	1:C:465:PHE:CE1	2.32	0.47
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.95	0.47
1:B:499:ASN:H	1:D:444:GLN:HE22	1.63	0.47
1:E:268:GLU:OE2	1:E:476:GLU:HG3	2.14	0.47
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.49	0.47
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.49	0.47
1:D:298:GLN:HB2	1:D:300:GLN:NE2	2.30	0.47
1:E:12:ASN:O	1:E:15:PRO:HD3	2.14	0.47
1:B:99:ARG:HG2	1:B:118:TYR:CE1	2.50	0.46
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.50	0.46
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.50	0.46
1:D:26:ASN:HD22	1:D:215:PRO:HG3	1.79	0.46
1:D:125:VAL:HG22	1:D:173:LEU:HA	1.98	0.46
1:D:196:GLN:H	1:D:196:GLN:NE2	2.10	0.46
1:B:404:VAL:HG12	1:B:406:GLN:OE1	2.15	0.46
1:H:39:THR:HG23	1:H:48:ILE:HB	1.98	0.46
1:H:205:ALA:HA	1:H:208:ILE:HD12	1.96	0.46
1:H:235:HIS:HB3	1:H:238:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:SER:HA	1:F:451:VAL:HG11	1.96	0.46
1:B:178:LYS:HE3	1:B:242:ALA:HB1	1.98	0.46
1:E:294:LEU:HD23	1:E:306:SER:HA	1.98	0.46
1:G:443:SER:HA	1:G:451:VAL:HG11	1.98	0.46
1:H:389:VAL:HB	1:H:408:LEU:HG	1.98	0.46
1:H:498:LYS:HG2	1:H:499:ASN:N	2.30	0.46
1:E:413:ILE:O	1:E:417:VAL:HG23	2.16	0.45
1:F:347:GLU:HG2	1:F:351:LYS:HE2	1.98	0.45
1:F:359:THR:O	1:F:363:GLU:HG2	2.17	0.45
1:F:459:PHE:HE2	1:F:465:PHE:CE1	2.34	0.45
1:G:275:ASN:HD22	1:G:430:ALA:HB3	1.81	0.45
1:D:149:ASP:HA	1:D:498:LYS:HB2	1.98	0.45
1:E:195:GLU:HG2	4:E:5575:HOH:O	2.15	0.45
1:D:159:VAL:HG11	1:D:240:LYS:HB2	1.99	0.45
1:D:449:GLY:HA3	1:D:466:GLY:O	2.17	0.45
1:D:275:ASN:ND2	1:D:430:ALA:HB3	2.32	0.45
1:B:443:SER:HA	1:B:451:VAL:HG11	1.97	0.45
1:H:172:LEU:HD21	1:H:200:THR:HB	1.98	0.45
1:H:432:PHE:HA	1:H:454:ASN:OD1	2.17	0.45
1:A:449:GLY:HA3	1:A:466:GLY:O	2.17	0.45
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.51	0.45
1:E:21:GLN:HB3	1:E:29:HIS:O	2.17	0.45
1:G:196:GLN:HE21	1:G:196:GLN:N	2.06	0.45
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.98	0.44
1:A:395:ILE:HG12	4:A:1754:HOH:O	2.17	0.44
1:D:272:LYS:HD2	1:D:306:SER:OG	2.17	0.44
1:E:449:GLY:HA3	1:E:466:GLY:O	2.17	0.44
1:H:170:PHE:HB3	1:H:173:LEU:HB3	1.99	0.44
1:F:143:THR:OG1	1:G:141:GLY:HA3	2.17	0.44
1:H:166:ILE:HD11	1:H:193:VAL:HG12	1.99	0.44
1:E:149:ASP:HA	1:E:498:LYS:HB2	2.00	0.44
1:E:417:VAL:HG22	1:E:442:LEU:HD23	1.98	0.44
1:G:158:PRO:HG3	1:G:185:THR:O	2.18	0.44
1:H:291:HIS:CE1	1:H:329:ARG:HD2	2.52	0.44
1:A:295:PHE:HE1	1:A:405:MET:CE	2.31	0.44
1:B:499:ASN:H	1:D:444:GLN:NE2	2.15	0.44
1:G:449:GLY:HA3	1:G:466:GLY:O	2.17	0.44
1:G:462:GLN:HB3	1:H:144:ILE:CG2	2.48	0.44
1:E:272:LYS:HD2	1:E:306:SER:OG	2.17	0.44
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.18	0.44
1:H:165:ILE:HG22	3:H:8502:NAD:H4B	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HD11	1:A:193:VAL:HG12	2.00	0.43
1:D:389:VAL:HB	1:D:408:LEU:HG	1.99	0.43
1:D:443:SER:HA	1:D:451:VAL:HG11	1.99	0.43
1:E:443:SER:HA	1:E:451:VAL:HG11	2.00	0.43
1:H:22:ILE:HG12	1:H:222:PRO:HD2	1.99	0.43
1:H:102:LEU:HD21	1:H:203:TYR:CD2	2.49	0.43
1:A:238:VAL:O	1:A:263:LYS:HE3	2.17	0.43
1:B:205:ALA:HB2	1:B:220:ILE:CD1	2.47	0.43
1:C:310:VAL:HG21	1:C:318:PHE:CD2	2.53	0.43
1:D:294:LEU:HD23	1:D:306:SER:HA	1.99	0.43
1:H:408:LEU:HD12	1:H:408:LEU:N	2.33	0.43
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.89	0.43
1:F:15:PRO:HG2	1:F:108:LEU:HD22	2.01	0.43
1:H:193:VAL:HG11	1:H:201:ALA:CB	2.49	0.43
1:A:149:ASP:HA	1:A:498:LYS:HB2	2.00	0.43
1:B:348:THR:O	1:B:352:LYS:HG3	2.19	0.43
1:D:12:ASN:O	1:D:15:PRO:HD3	2.18	0.43
1:F:494:LYS:HE3	4:H:8619:HOH:O	2.19	0.43
1:B:449:GLY:HA3	1:B:466:GLY:O	2.19	0.43
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.84	0.43
1:D:332:GLY:O	1:D:380:PHE:HE2	2.02	0.43
1:F:135:TRP:CD1	1:H:138:LYS:HE3	2.54	0.43
1:E:323:VAL:O	1:E:327:LYS:HG3	2.18	0.43
1:F:283:MET:CE	1:F:318:PHE:HD1	2.32	0.43
1:H:15:PRO:HG2	1:H:108:LEU:HD22	2.01	0.43
1:A:410:PHE:CD1	1:A:416:VAL:HB	2.54	0.42
1:E:408:LEU:N	1:E:408:LEU:HD12	2.34	0.42
1:H:294:LEU:HD23	1:H:306:SER:HA	2.00	0.42
1:B:113:PRO:HB2	1:B:116:ILE:HG12	2.01	0.42
1:B:159:VAL:HG12	1:B:187:ASN:OD1	2.19	0.42
1:B:183:LEU:HD13	1:B:213:PHE:CE2	2.53	0.42
1:G:248:GLU:HG3	4:G:7603:HOH:O	2.19	0.42
1:G:249:ILE:O	1:G:253:ILE:HG12	2.19	0.42
1:H:214:PRO:HA	1:H:215:PRO:HD3	1.88	0.42
1:H:449:GLY:HA3	1:H:466:GLY:O	2.19	0.42
1:C:449:GLY:HA3	1:C:466:GLY:O	2.19	0.42
1:E:389:VAL:HB	1:E:408:LEU:HG	2.01	0.42
1:H:13:GLN:HA	1:H:335:PHE:CZ	2.55	0.42
1:D:21:GLN:HB3	1:D:29:HIS:O	2.19	0.42
1:E:34:ARG:HE	1:E:34:ARG:HB3	1.27	0.42
1:G:238:VAL:O	1:G:263:LYS:HE3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:GLN:O	1:H:353:ILE:HG13	2.19	0.42
1:B:442:LEU:O	1:B:446:LEU:HG	2.19	0.42
1:C:241:VAL:HG13	1:C:265:VAL:HG22	2.02	0.42
1:G:247:THR:HA	1:G:269:LEU:HD13	2.01	0.42
1:H:466:GLY:HA3	1:H:475:ARG:HD3	2.01	0.42
1:A:113:PRO:HB2	1:A:116:ILE:HG12	2.01	0.42
1:A:430:ALA:HB2	1:A:456:TYR:CD1	2.55	0.42
1:C:291:HIS:HD2	4:C:3594:HOH:O	2.02	0.42
1:C:303:CYS:SG	1:C:459:PHE:HZ	2.42	0.42
1:E:372:GLY:O	1:E:382:GLN:HG3	2.20	0.42
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.19	0.42
1:H:413:ILE:O	1:H:416:VAL:HG12	2.19	0.42
1:B:333:ASN:HB3	1:B:336:ASP:OD2	2.20	0.42
1:C:443:SER:HA	1:C:451:VAL:HG11	2.02	0.42
1:E:167:PRO:HD3	1:E:244:THR:HB	2.02	0.42
1:G:86:ARG:HD2	4:G:7619:HOH:O	2.19	0.42
1:C:372:GLY:O	1:C:382:GLN:HG3	2.20	0.41
1:F:283:MET:HA	1:F:283:MET:CE	2.44	0.41
1:G:59:VAL:O	1:G:63:VAL:HG23	2.20	0.41
1:A:368:LEU:HD12	1:A:385:VAL:HG12	2.02	0.41
1:E:279:SER:HA	1:E:314:ILE:HD13	2.03	0.41
1:H:32:VAL:HG23	1:H:58:ASP:OD1	2.20	0.41
1:H:158:PRO:HG3	1:H:185:THR:O	2.20	0.41
1:D:41:ASN:HD22	1:D:43:SER:H	1.66	0.41
1:E:46:GLU:CD	1:E:377:ARG:NH2	2.73	0.41
1:H:333:ASN:HA	1:H:334:PRO:HD2	1.94	0.41
1:C:333:ASN:HA	1:C:334:PRO:HD2	1.95	0.41
1:D:464:PRO:HA	1:D:476:GLU:O	2.20	0.41
1:F:352:LYS:HB2	1:F:352:LYS:HE3	1.76	0.41
1:G:111:GLY:O	1:G:343:PRO:HD2	2.20	0.41
1:B:421:ASN:CG	1:B:447:GLN:HG3	2.40	0.41
1:F:111:GLY:O	1:F:343:PRO:HD2	2.21	0.41
1:G:476:GLU:O	1:G:477:LEU:HB2	2.20	0.41
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.94	0.41
1:A:498:LYS:HD2	1:A:498:LYS:C	2.42	0.41
1:F:193:VAL:HG11	1:F:201:ALA:CB	2.51	0.41
1:G:351:LYS:HB3	1:G:351:LYS:HE2	1.90	0.41
1:F:21:GLN:HB3	1:F:29:HIS:O	2.21	0.41
1:C:476:GLU:O	1:C:477:LEU:HB2	2.21	0.40
1:D:214:PRO:HA	1:D:215:PRO:HD3	1.91	0.40
1:F:238:VAL:O	1:F:263:LYS:HE3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:GLU:O	1:F:477:LEU:HB2	2.21	0.40
1:H:464:PRO:HA	1:H:476:GLU:O	2.21	0.40
1:H:498:LYS:HE2	1:H:498:LYS:HB3	1.95	0.40
1:A:408:LEU:HD12	1:A:408:LEU:N	2.36	0.40
1:C:431:VAL:HG21	1:C:442:LEU:HB3	2.03	0.40
1:D:169:ASN:ND2	1:D:170:PHE:CD1	2.88	0.40
1:G:185:THR:HG23	1:G:482:LEU:HD22	2.02	0.40
1:C:23:PHE:HB2	1:C:28:TRP:CZ3	2.56	0.40
1:D:172:LEU:HD21	1:D:200:THR:HB	2.02	0.40
1:H:196:GLN:OE1	1:H:196:GLN:N	2.54	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	492/500 (98%)	475 (96%)	17 (4%)	0	100	100
1	B	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	C	492/500 (98%)	475 (96%)	17 (4%)	0	100	100
1	D	492/500 (98%)	475 (96%)	16 (3%)	1 (0%)	47	57
1	E	492/500 (98%)	474 (96%)	17 (4%)	1 (0%)	47	57
1	F	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	G	492/500 (98%)	478 (97%)	13 (3%)	1 (0%)	47	57
1	H	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
All	All	3936/4000 (98%)	3802 (97%)	131 (3%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	13	GLN
1	E	426	GLY
1	G	426	GLY

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	399/402 (99%)	394 (99%)	5 (1%)	69	79
1	B	399/402 (99%)	396 (99%)	3 (1%)	81	88
1	C	399/402 (99%)	397 (100%)	2 (0%)	88	93
1	D	399/402 (99%)	394 (99%)	5 (1%)	69	79
1	E	399/402 (99%)	395 (99%)	4 (1%)	76	84
1	F	399/402 (99%)	395 (99%)	4 (1%)	76	84
1	G	399/402 (99%)	395 (99%)	4 (1%)	76	84
1	H	399/402 (99%)	396 (99%)	3 (1%)	81	88
All	All	3192/3216 (99%)	3162 (99%)	30 (1%)	78	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	275	ASN
1	A	333	ASN
1	A	401	PHE
1	A	408	LEU
1	B	192	LYS
1	B	401	PHE
1	B	422	ASN
1	C	192	LYS
1	C	401	PHE
1	D	41	ASN
1	D	192	LYS
1	D	196	GLN

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Mol	Chain	Res	Type
1	D	377	ARG
1	D	401	PHE
1	E	34	ARG
1	E	192	LYS
1	E	206	ASN
1	E	401	PHE
1	F	192	LYS
1	F	376	ASP
1	F	401	PHE
1	F	498	LYS
1	G	192	LYS
1	G	196	GLN
1	G	401	PHE
1	G	422	ASN
1	H	121	ASP
1	H	192	LYS
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	275	ASN
1	A	333	ASN
1	B	83	HIS
1	B	175	GLN
1	B	275	ASN
1	B	422	ASN
1	B	440	ASN
1	C	13	GLN
1	C	175	GLN
1	C	291	HIS
1	C	483	GLN
1	D	13	GLN
1	D	26	ASN
1	D	41	ASN
1	D	89	ASN
1	D	140	HIS
1	D	196	GLN
1	D	275	ASN
1	D	289	GLN
1	D	444	GLN

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Mol	Chain	Res	Type
1	E	83	HIS
1	E	164	GLN
1	E	440	ASN
1	E	483	GLN
1	F	21	GLN
1	F	29	HIS
1	F	175	GLN
1	G	13	GLN
1	G	196	GLN
1	G	275	ASN
1	G	362	GLN
1	G	422	ASN
1	H	13	GLN
1	H	291	HIS
1	H	390	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	E	5502	-	24,29,48	1.61	4 (16%)	29,45,73	1.59	4 (13%)
3	NAD	C	3502	-	24,29,48	1.54	4 (16%)	29,45,73	1.44	4 (13%)
3	NAD	G	7502	-	24,29,48	1.54	4 (16%)	29,45,73	1.56	4 (13%)
3	NAD	H	8502	-	24,29,48	1.70	5 (20%)	29,45,73	1.73	5 (17%)
3	NAD	B	2502	-	24,29,48	1.62	4 (16%)	29,45,73	1.46	4 (13%)
3	NAD	A	1502	-	24,29,48	1.66	5 (20%)	29,45,73	1.53	4 (13%)
3	NAD	D	4502	-	24,29,48	1.57	4 (16%)	29,45,73	1.50	4 (13%)
3	NAD	F	6502	-	24,29,48	1.61	4 (16%)	29,45,73	1.56	4 (13%)

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	E	5502	-	-	1/12/32/62	0/3/3/5
3	NAD	C	3502	-	-	1/12/32/62	0/3/3/5
3	NAD	G	7502	-	-	2/12/32/62	0/3/3/5
3	NAD	H	8502	-	-	1/12/32/62	0/3/3/5
3	NAD	B	2502	-	-	1/12/32/62	0/3/3/5
3	NAD	A	1502	-	-	1/12/32/62	0/3/3/5
3	NAD	D	4502	-	-	1/12/32/62	0/3/3/5
3	NAD	F	6502	-	-	1/12/32/62	0/3/3/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8502	NAD	C2A-N3A	4.79	1.39	1.32
3	A	1502	NAD	C2A-N3A	4.74	1.39	1.32
3	F	6502	NAD	C2A-N3A	4.65	1.39	1.32
3	B	2502	NAD	C2A-N3A	4.64	1.39	1.32
3	E	5502	NAD	C2A-N3A	4.57	1.39	1.32
3	D	4502	NAD	C2A-N3A	4.42	1.39	1.32
3	C	3502	NAD	C2A-N3A	4.37	1.39	1.32
3	G	7502	NAD	C2A-N3A	4.23	1.38	1.32
3	E	5502	NAD	C8A-N7A	3.38	1.40	1.34
3	G	7502	NAD	C2A-N1A	3.36	1.40	1.33
3	F	6502	NAD	C2A-N1A	3.30	1.40	1.33
3	H	8502	NAD	C2A-N1A	3.18	1.39	1.33
3	A	1502	NAD	C2A-N1A	3.17	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6502	NAD	C8A-N7A	3.10	1.40	1.34
3	H	8502	NAD	C8A-N7A	2.99	1.40	1.34
3	H	8502	NAD	PN-O5D	2.95	1.66	1.54
3	B	2502	NAD	C2A-N1A	2.95	1.39	1.33
3	B	2502	NAD	C8A-N7A	2.95	1.39	1.34
3	D	4502	NAD	C2A-N1A	2.92	1.39	1.33
3	A	1502	NAD	C8A-N7A	2.89	1.39	1.34
3	E	5502	NAD	C2A-N1A	2.86	1.39	1.33
3	D	4502	NAD	C8A-N7A	2.86	1.39	1.34
3	C	3502	NAD	C8A-N7A	2.85	1.39	1.34
3	B	2502	NAD	PN-O5D	2.85	1.65	1.54
3	C	3502	NAD	C2A-N1A	2.70	1.38	1.33
3	G	7502	NAD	C8A-N7A	2.56	1.39	1.34
3	F	6502	NAD	PN-O5D	2.55	1.64	1.54
3	C	3502	NAD	PN-O5D	2.54	1.64	1.54
3	H	8502	NAD	C4A-N3A	2.45	1.39	1.35
3	E	5502	NAD	PN-O5D	2.45	1.64	1.54
3	G	7502	NAD	PN-O5D	2.41	1.64	1.54
3	A	1502	NAD	PN-O5D	2.40	1.64	1.54
3	A	1502	NAD	C4A-N3A	2.37	1.38	1.35
3	D	4502	NAD	PN-O5D	2.33	1.63	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	8502	NAD	O4B-C1B-C2B	-5.01	99.61	106.93
3	G	7502	NAD	O4B-C1B-C2B	-4.62	100.18	106.93
3	E	5502	NAD	O4B-C1B-C2B	-4.44	100.43	106.93
3	F	6502	NAD	O4B-C1B-C2B	-4.44	100.44	106.93
3	A	1502	NAD	O4B-C1B-C2B	-4.22	100.77	106.93
3	C	3502	NAD	O4B-C1B-C2B	-4.10	100.93	106.93
3	D	4502	NAD	O4B-C1B-C2B	-4.10	100.93	106.93
3	H	8502	NAD	N3A-C2A-N1A	-4.00	122.42	128.68
3	E	5502	NAD	N3A-C2A-N1A	-4.00	122.42	128.68
3	A	1502	NAD	N3A-C2A-N1A	-3.87	122.64	128.68
3	H	8502	NAD	C2B-C3B-C4B	-3.80	95.25	102.64
3	G	7502	NAD	N3A-C2A-N1A	-3.78	122.77	128.68
3	D	4502	NAD	N3A-C2A-N1A	-3.73	122.85	128.68
3	B	2502	NAD	O4B-C1B-C2B	-3.72	101.48	106.93
3	B	2502	NAD	N3A-C2A-N1A	-3.69	122.91	128.68
3	C	3502	NAD	N3A-C2A-N1A	-3.63	123.00	128.68
3	F	6502	NAD	N3A-C2A-N1A	-3.55	123.13	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	6502	NAD	PA-O3-PN	-3.49	120.85	132.83
3	C	3502	NAD	PA-O3-PN	-3.48	120.90	132.83
3	E	5502	NAD	C2B-C3B-C4B	-3.44	95.95	102.64
3	A	1502	NAD	C2B-C3B-C4B	-3.35	96.13	102.64
3	D	4502	NAD	C2B-C3B-C4B	-3.16	96.50	102.64
3	H	8502	NAD	PA-O3-PN	-3.12	122.11	132.83
3	G	7502	NAD	PA-O3-PN	-3.07	122.28	132.83
3	F	6502	NAD	C2B-C3B-C4B	-3.07	96.67	102.64
3	G	7502	NAD	C2B-C3B-C4B	-3.07	96.68	102.64
3	B	2502	NAD	C2B-C3B-C4B	-3.05	96.71	102.64
3	B	2502	NAD	PA-O3-PN	-2.97	122.62	132.83
3	D	4502	NAD	PA-O3-PN	-2.94	122.72	132.83
3	E	5502	NAD	PA-O3-PN	-2.80	123.21	132.83
3	A	1502	NAD	PA-O3-PN	-2.75	123.38	132.83
3	C	3502	NAD	O5B-C5B-C4B	2.15	116.40	108.99
3	H	8502	NAD	O4B-C4B-C3B	2.09	109.25	105.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	7502	NAD	C5B-O5B-PA-O1A
3	G	7502	NAD	C5B-O5B-PA-O3
3	A	1502	NAD	C5B-O5B-PA-O1A
3	B	2502	NAD	C5B-O5B-PA-O1A
3	C	3502	NAD	C5B-O5B-PA-O1A
3	D	4502	NAD	C5B-O5B-PA-O1A
3	E	5502	NAD	C5B-O5B-PA-O1A
3	F	6502	NAD	C5B-O5B-PA-O1A
3	H	8502	NAD	C5B-O5B-PA-O1A

There are no ring outliers.

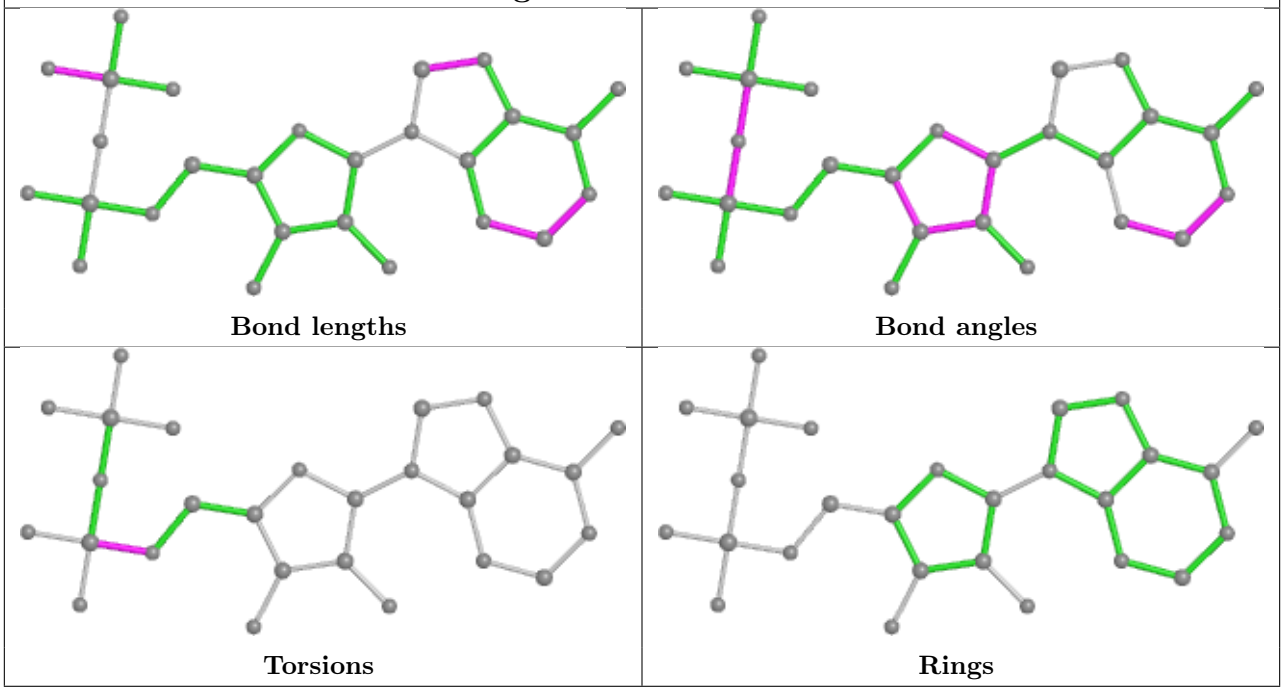
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	8502	NAD	1	0

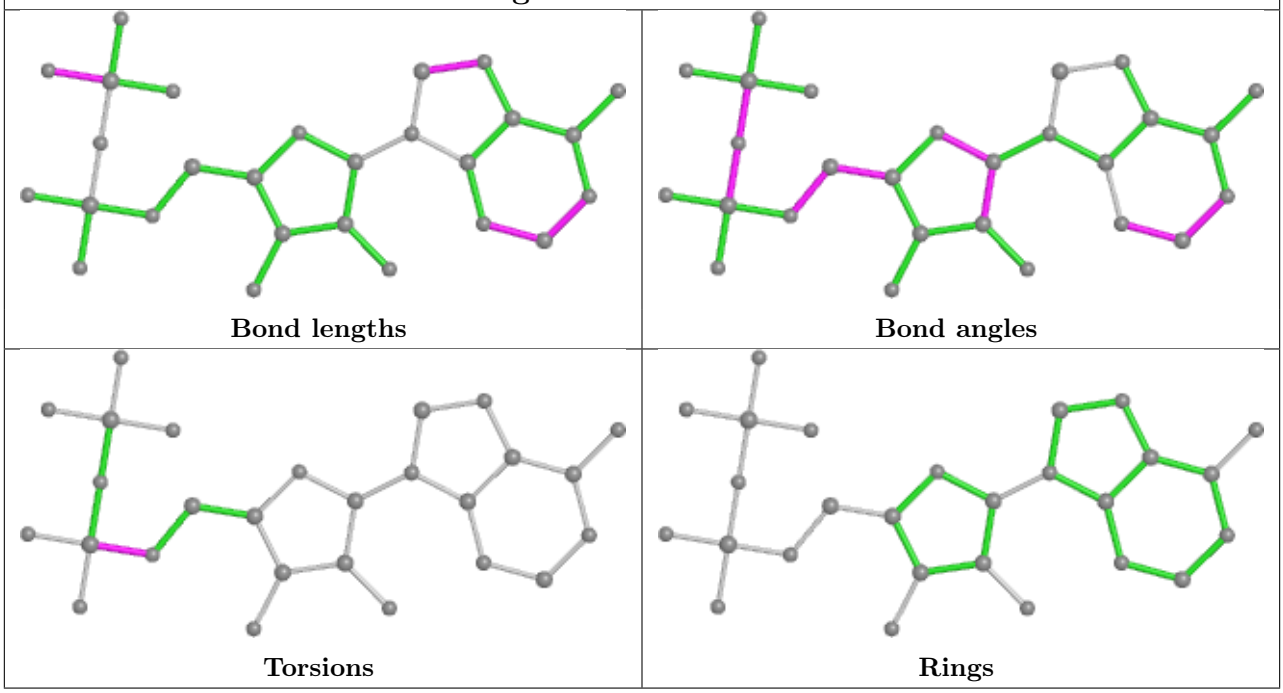
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

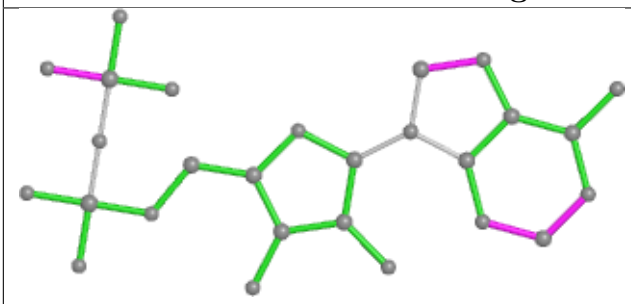
Ligand NAD E 5502



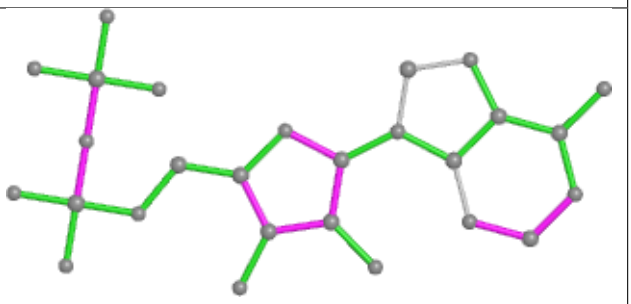
Ligand NAD C 3502



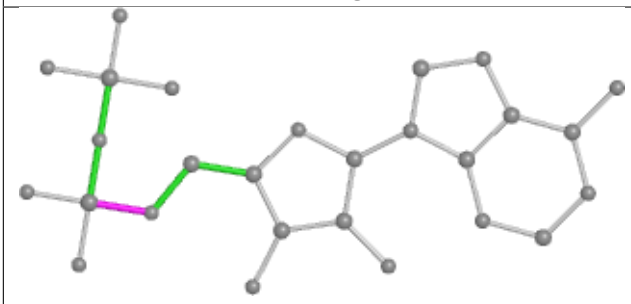
Ligand NAD G 7502



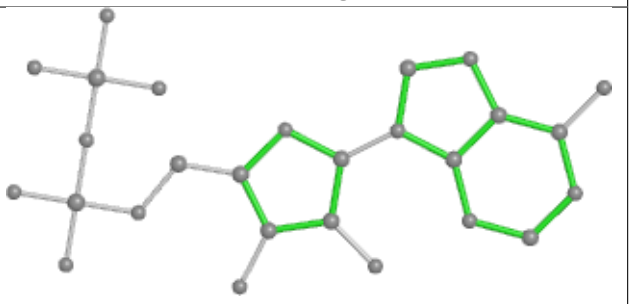
Bond lengths



Bond angles

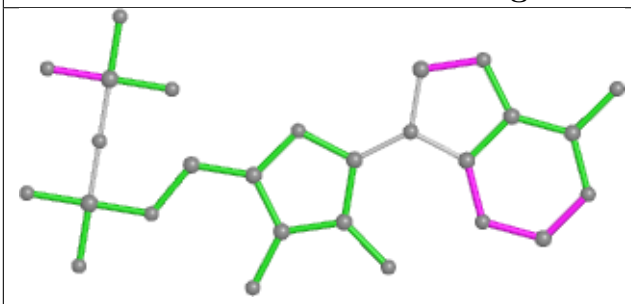


Torsions

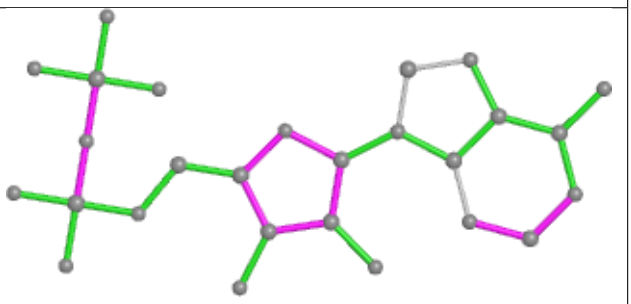


Rings

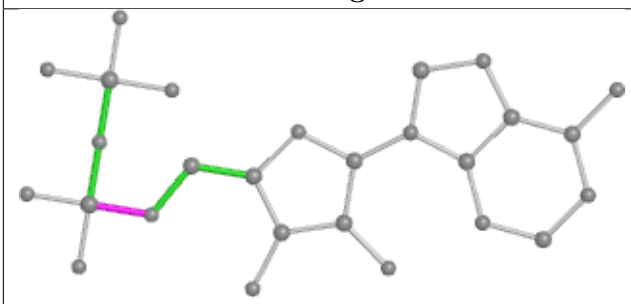
Ligand NAD H 8502



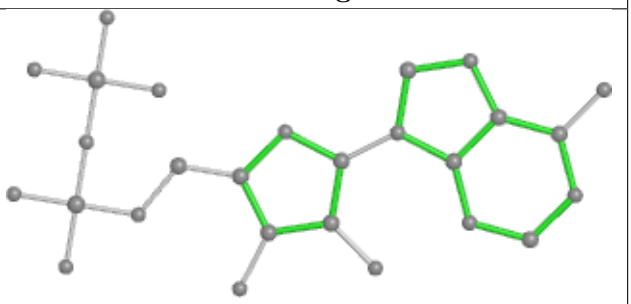
Bond lengths



Bond angles

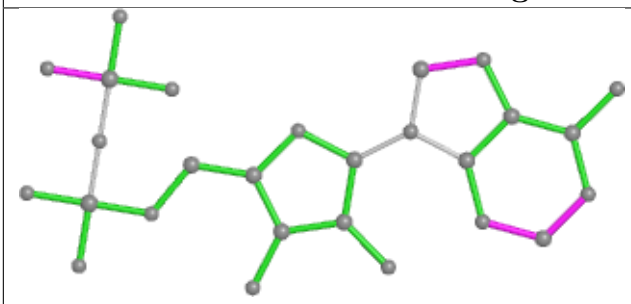


Torsions

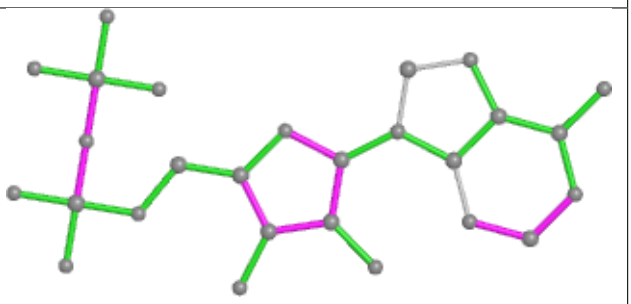


Rings

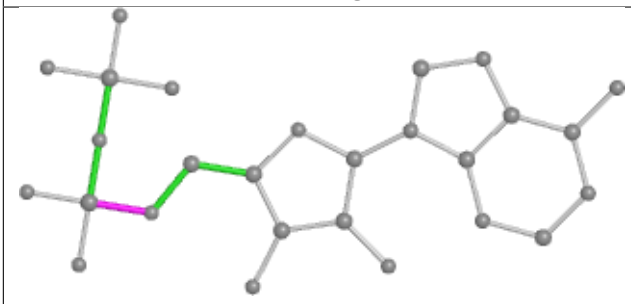
Ligand NAD B 2502



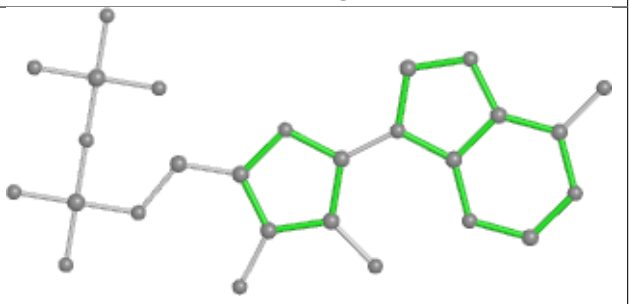
Bond lengths



Bond angles

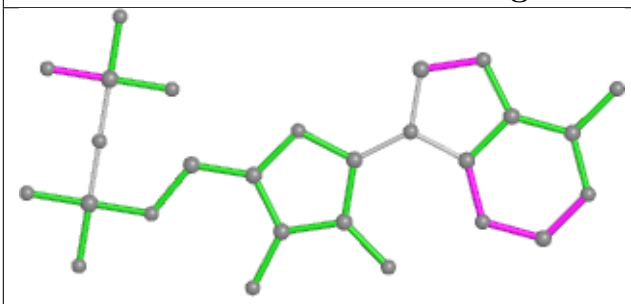


Torsions

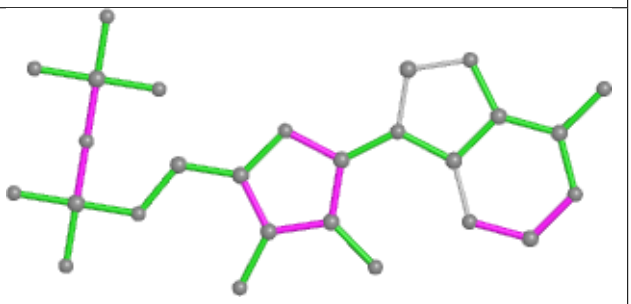


Rings

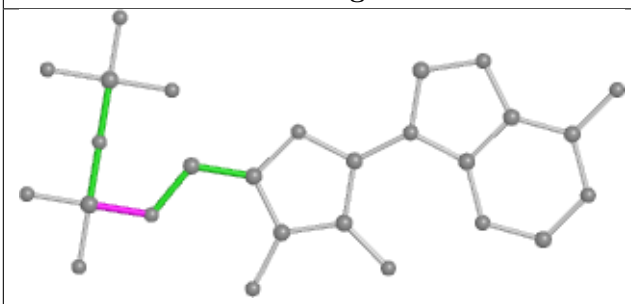
Ligand NAD A 1502



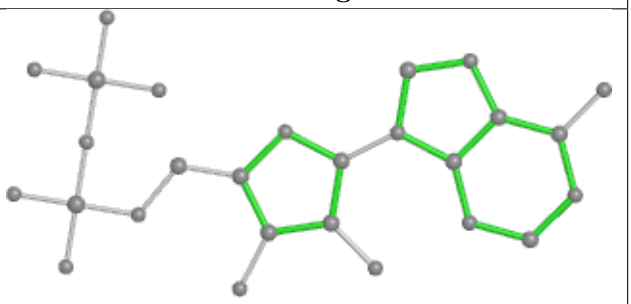
Bond lengths



Bond angles

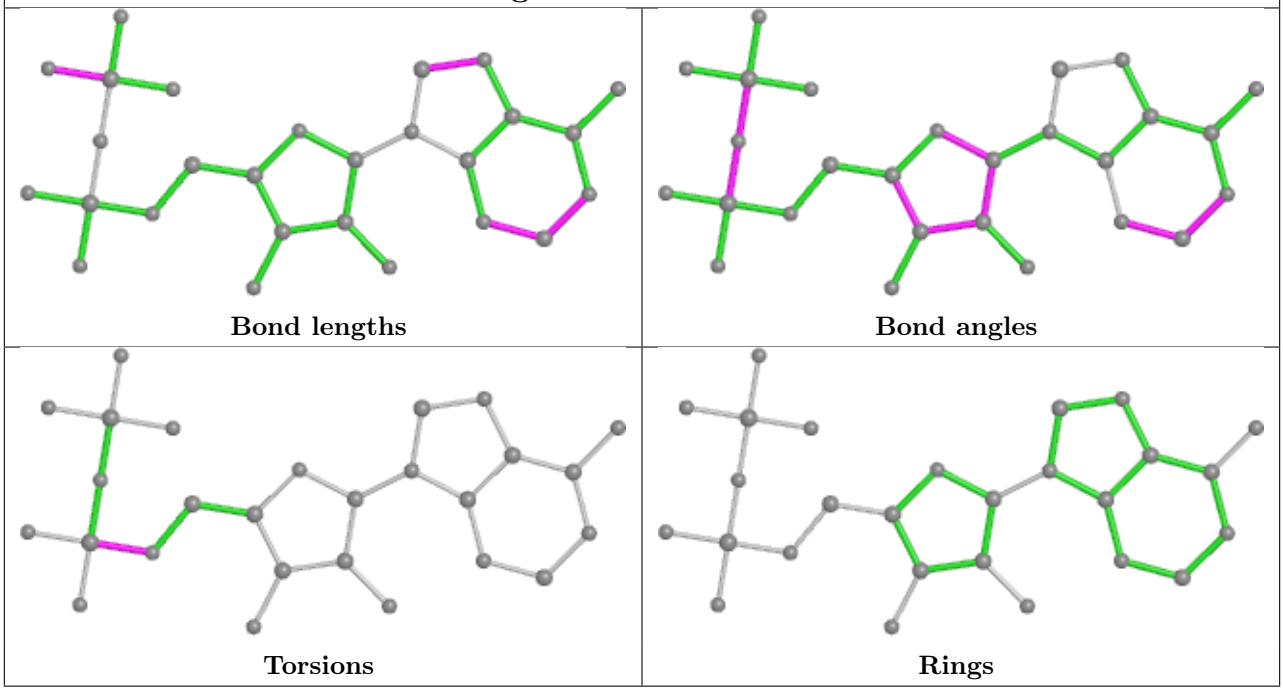


Torsions

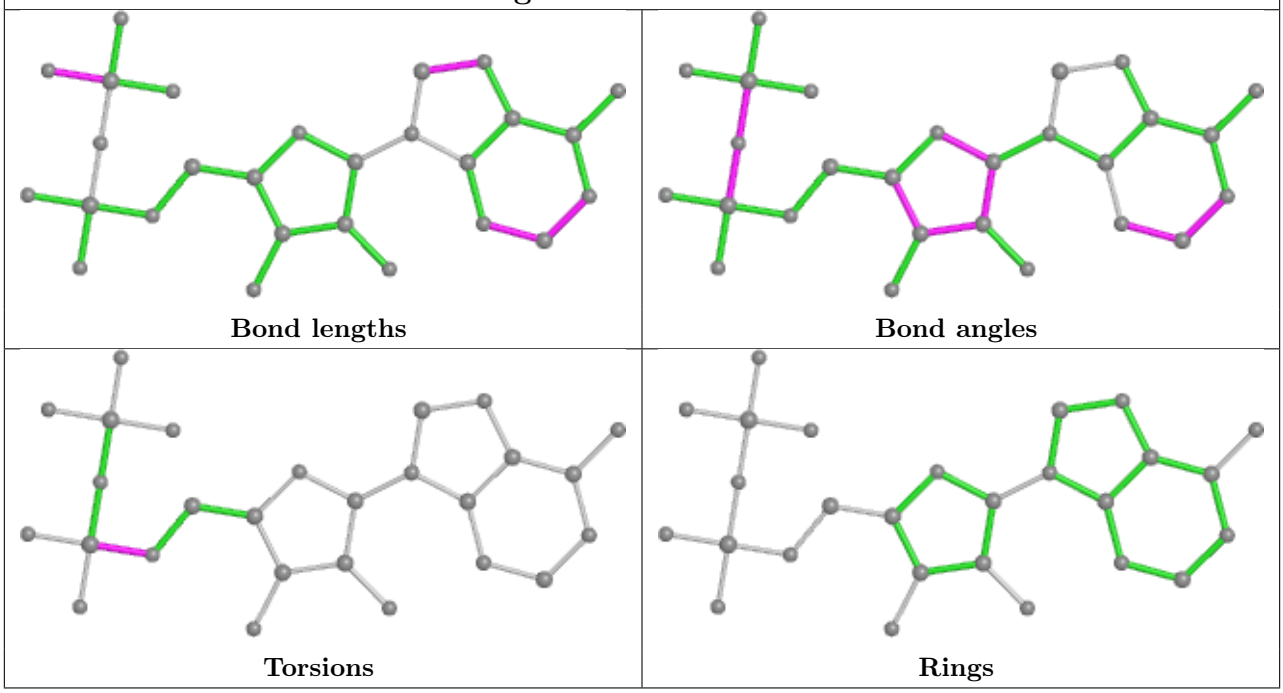


Rings

Ligand NAD D 4502



Ligand NAD F 6502



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	494/500 (98%)	-0.14	10 (2%)	65	62	14, 33, 47, 59	0
1	B	494/500 (98%)	-0.37	4 (0%)	86	86	16, 29, 42, 52	0
1	C	494/500 (98%)	-0.48	1 (0%)	95	95	13, 26, 38, 48	0
1	D	494/500 (98%)	0.07	13 (2%)	56	52	16, 38, 53, 60	0
1	E	494/500 (98%)	-0.40	2 (0%)	92	93	13, 28, 42, 56	0
1	F	494/500 (98%)	-0.57	4 (0%)	86	86	14, 24, 35, 48	0
1	G	494/500 (98%)	-0.40	4 (0%)	86	86	15, 29, 41, 52	0
1	H	494/500 (98%)	0.00	13 (2%)	56	52	14, 36, 49, 66	0
All	All	3952/4000 (98%)	-0.29	51 (1%)	77	76	13, 29, 47, 66	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	GLN	5.2
1	D	376	ASP	4.2
1	G	14	GLN	4.1
1	H	377	ARG	3.9
1	H	376	ASP	3.8
1	F	7	ALA	3.8
1	A	376	ASP	3.7
1	D	7	ALA	3.6
1	D	14	GLN	3.5
1	B	34	ARG	3.4
1	D	338	LYS	3.2
1	B	7	ALA	3.2
1	H	362	GLN	3.2
1	H	34	ARG	3.2
1	H	7	ALA	3.1
1	D	362	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	376	ASP	3.0
1	D	34	ARG	2.9
1	A	377	ARG	2.8
1	H	375	ALA	2.8
1	D	332	GLY	2.8
1	F	248	GLU	2.7
1	H	10	ALA	2.7
1	A	371	GLY	2.6
1	B	377	ARG	2.6
1	G	7	ALA	2.6
1	D	36	THR	2.6
1	F	338	LYS	2.6
1	H	51	VAL	2.6
1	H	338	LYS	2.5
1	A	392	GLY	2.4
1	G	34	ARG	2.4
1	D	224	PHE	2.3
1	H	394	THR	2.3
1	C	7	ALA	2.3
1	A	14	GLN	2.3
1	H	44	THR	2.3
1	E	34	ARG	2.3
1	F	14	GLN	2.3
1	D	107	THR	2.2
1	D	333	ASN	2.2
1	D	50	GLN	2.2
1	H	32	VAL	2.2
1	A	411	LYS	2.2
1	D	347	GLU	2.2
1	A	356	TYR	2.1
1	A	34	ARG	2.1
1	H	424	THR	2.1
1	B	32	VAL	2.1
1	A	277	ILE	2.1
1	G	226	PRO	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)

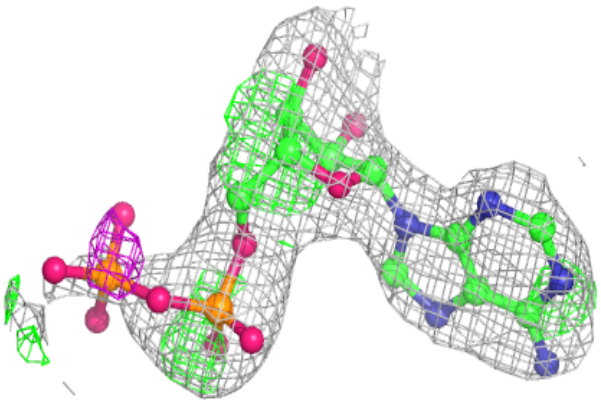
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

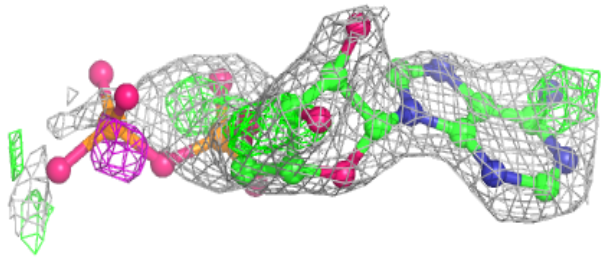
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	D	1704	1/1	0.43	0.49	95,95,95,95	0
2	NA	C	1703	1/1	0.59	0.55	55,55,55,55	0
2	NA	H	1708	1/1	0.60	0.42	55,55,55,55	0
3	NAD	H	8502	27/44	0.73	0.38	26,28,45,45	27
2	NA	E	1705	1/1	0.77	0.36	52,52,52,52	0
2	NA	A	1701	1/1	0.79	0.17	50,50,50,50	0
3	NAD	G	7502	27/44	0.80	0.32	20,23,35,36	27
3	NAD	A	1502	27/44	0.81	0.30	21,25,38,38	26
2	NA	G	1707	1/1	0.83	0.18	33,33,33,33	0
3	NAD	C	3502	27/44	0.83	0.30	9,15,34,35	27
3	NAD	B	2502	27/44	0.84	0.31	21,23,37,38	27
3	NAD	F	6502	27/44	0.86	0.27	5,11,27,28	27
2	NA	B	1702	1/1	0.86	0.35	44,44,44,44	0
3	NAD	E	5502	27/44	0.86	0.31	8,15,32,32	27
3	NAD	D	4502	27/44	0.87	0.33	19,27,36,38	27
2	NA	F	1706	1/1	0.95	0.27	39,39,39,39	0

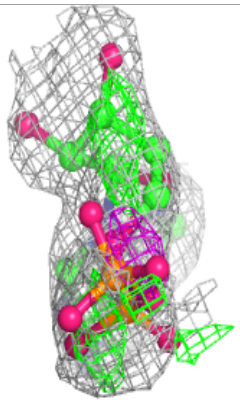
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD H 8502:

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

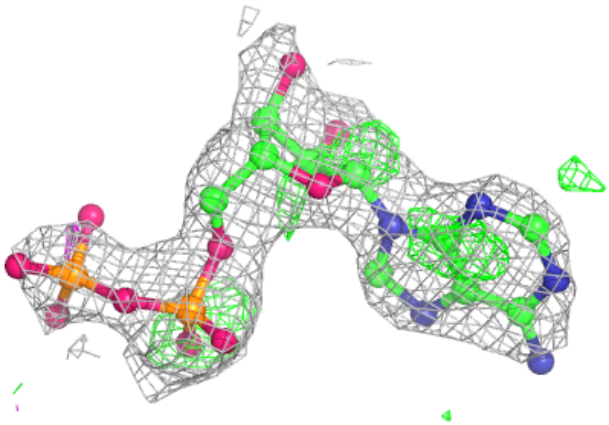


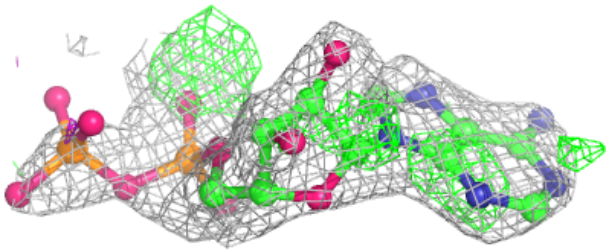


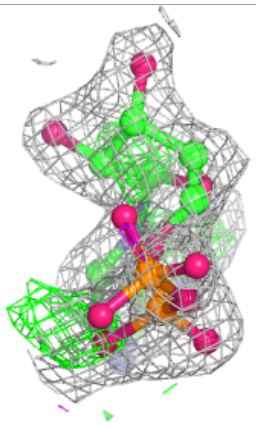


Electron density around NAD G 7502:

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

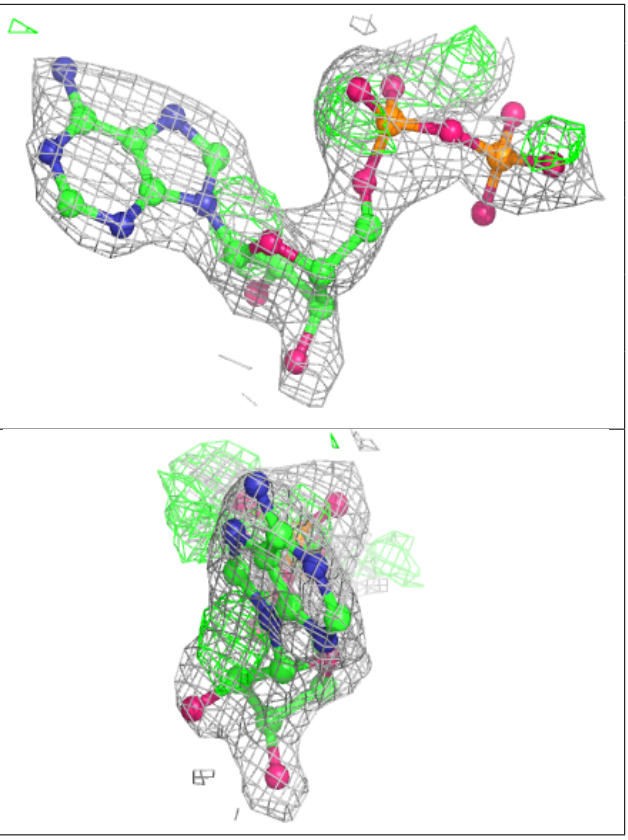


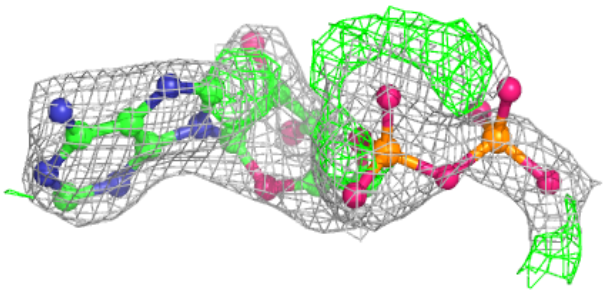




Electron density around NAD A 1502:

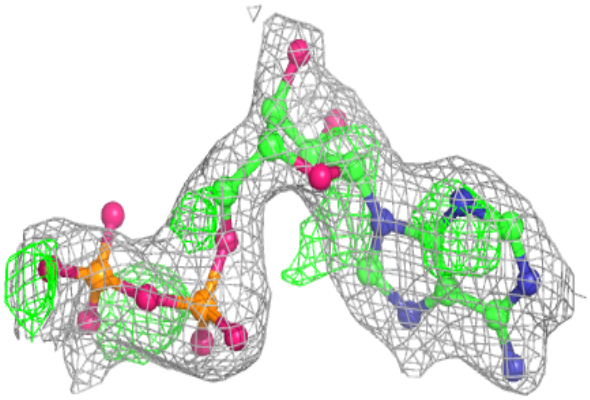
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

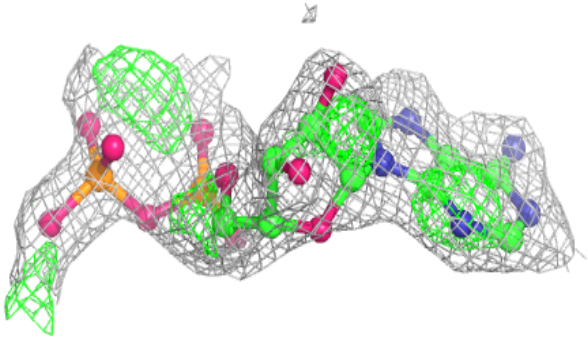


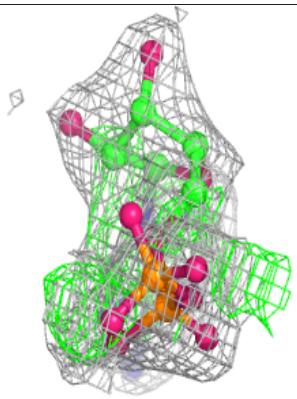


Electron density around NAD C 3502:

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

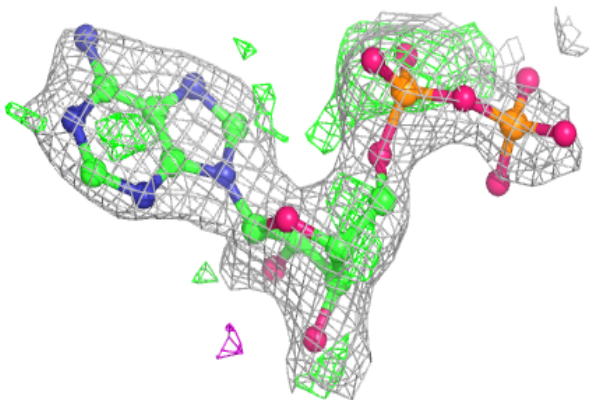


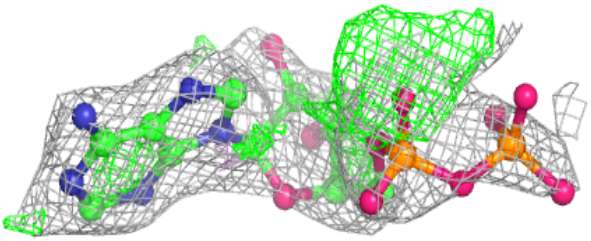


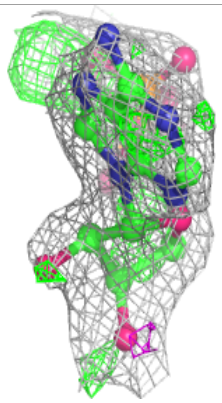


Electron density around NAD B 2502:

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

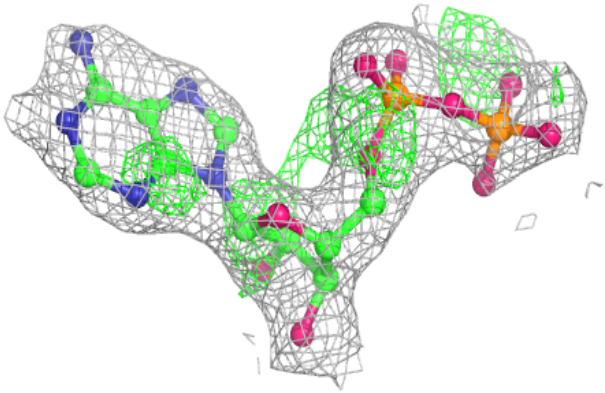


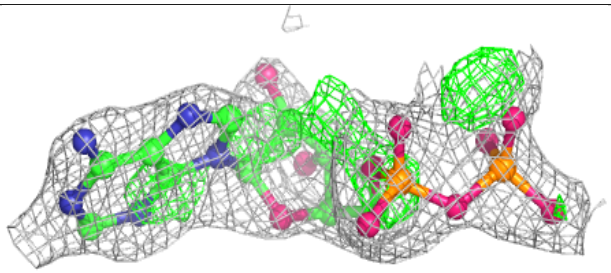


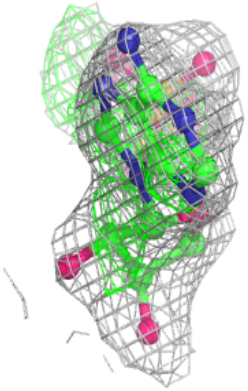


Electron density around NAD F 6502:

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

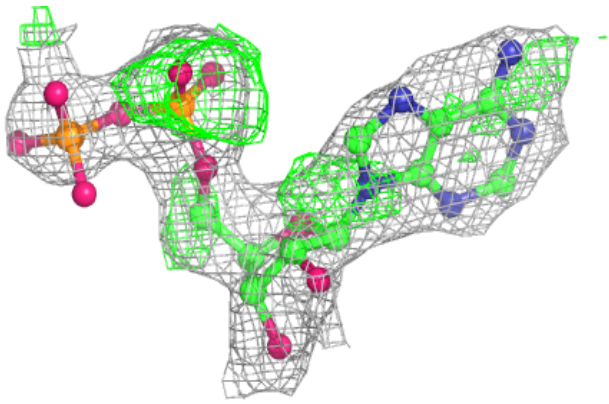


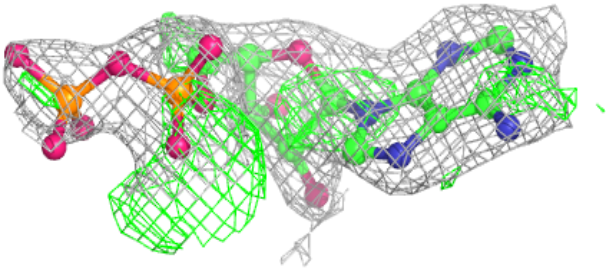


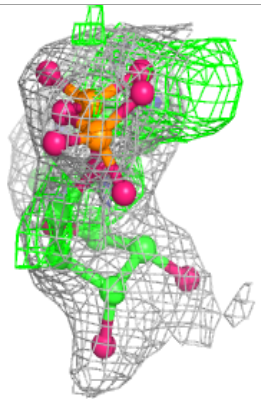


Electron density around NAD E 5502:

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

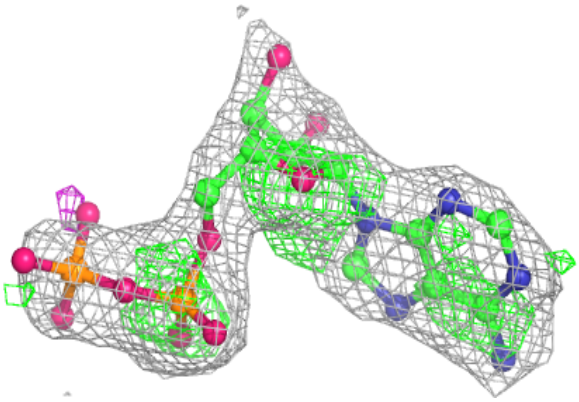


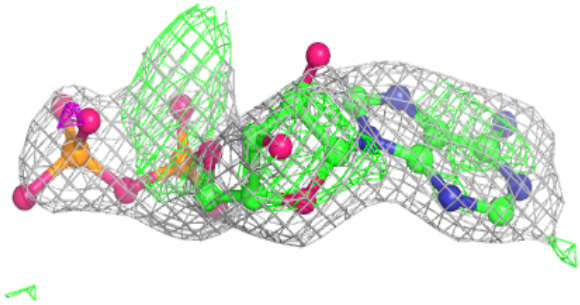


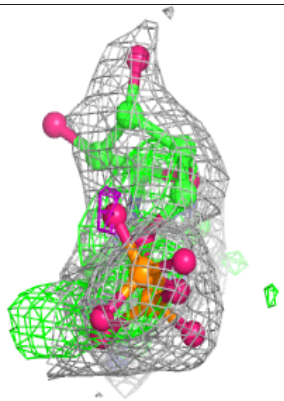


Electron density around NAD D 4502:

$2mF_o$-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.