Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 06:32 pm GMT

PDB ID	:	2V7P
Title	:	Crystal structure of lactate dehydrogenase from Thermus Thermophilus HB8 (Holo form)
Authors	:	Coquelle, N.; Fioravanti, E.; Weik, M.; Vellieux, F.
Deposited on	:	2007-07-31
Resolution	:	2.10 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:

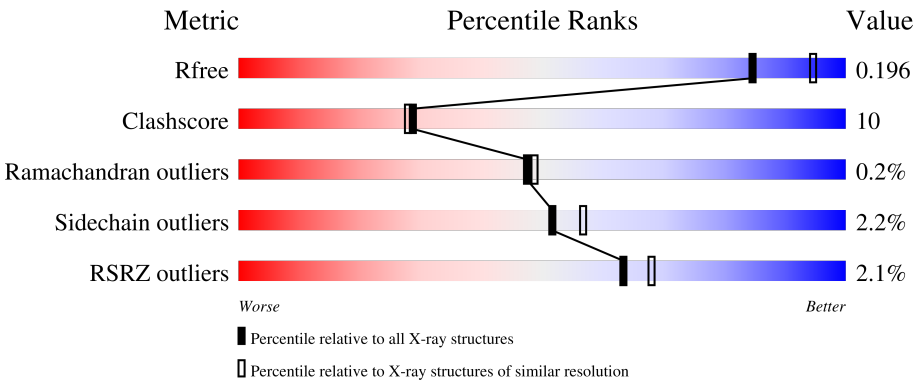
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	310	% 85% 14% •
1	B	310	4% 77% 17% • •
1	C	310	85% 14% •
1	D	310	3% 78% 18% • •

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	OXM	A	501	-	X	-	-
3	NAD	D	1332	X	-	-	-

2 Entry composition (i)

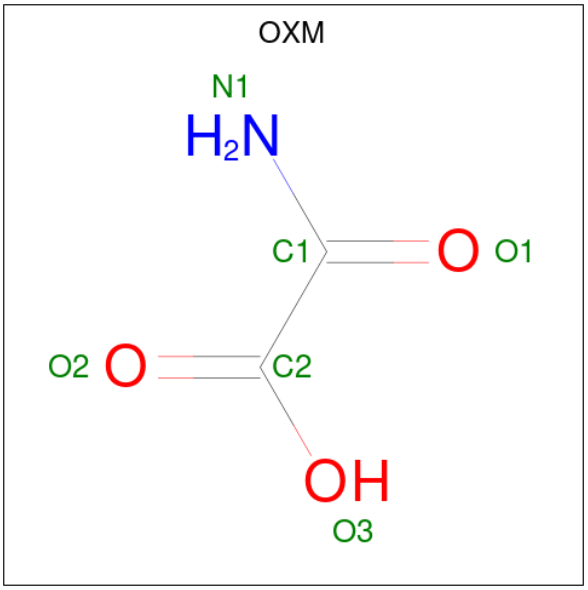
There are 4 unique types of molecules in this entry. The entry contains 9824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2324	1474	418	429	3	0	4	0
1	B	299	2234	1420	399	412	3	0	2	0
1	C	310	2319	1472	416	428	3	0	2	0
1	D	300	2212	1412	395	402	3	0	1	0

- Molecule 2 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	6	2	1	3	0	0
2	B	1	6	2	1	3	0	0

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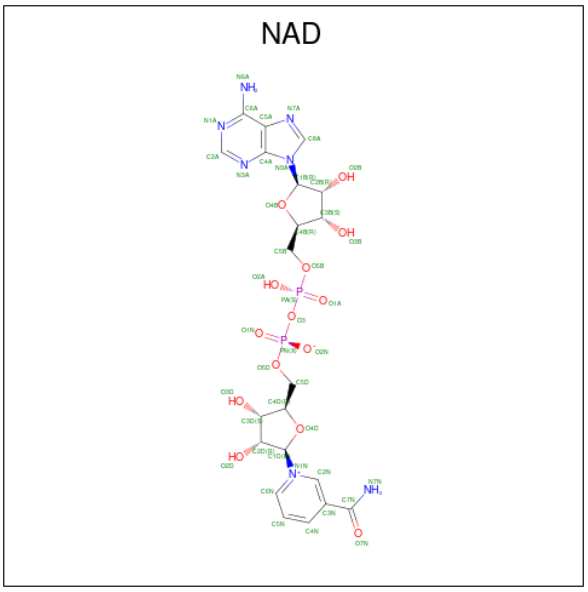
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	6	2	1	3	0	0
			Total	C	N	O		
2	D	1	6	2	1	3	0	0

- 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	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	B	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	C	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	D	1	44	21	7	14	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	147	147	147	0	0
			Total	O		
4	B	136	136	136	0	0
			Total	O		
4	C	152	152	152	0	0

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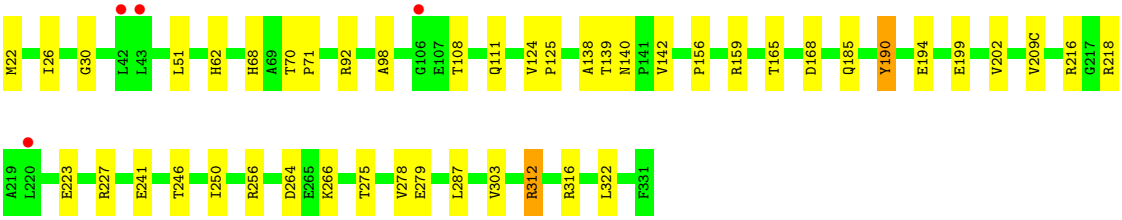
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	100	100	100	0	0

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.

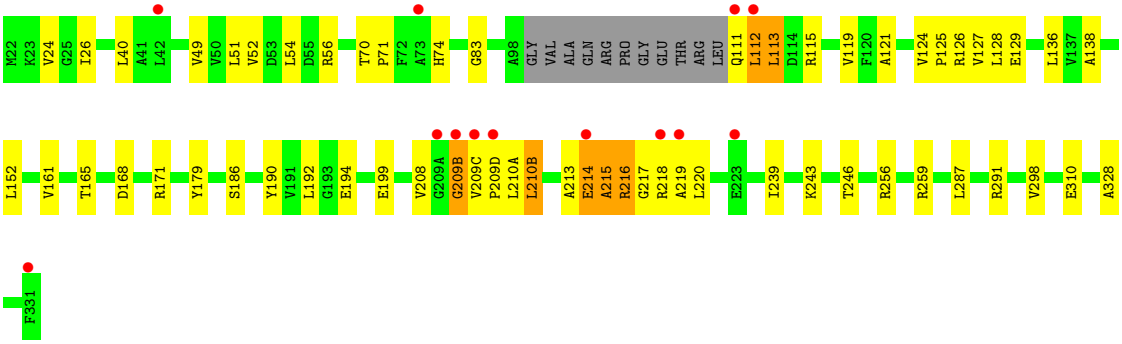
• Molecule 1: L-LACTATE DEHYDROGENASE

Chain A:



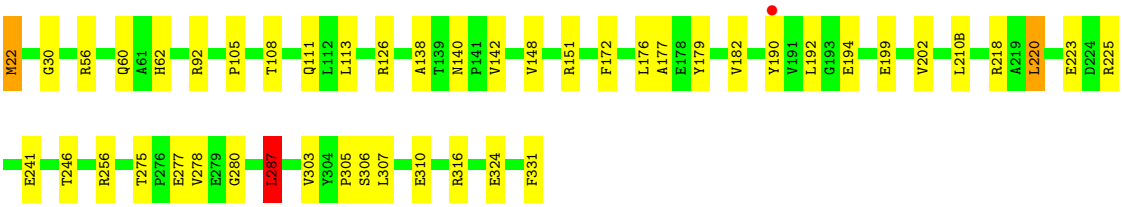
• Molecule 1: L-LACTATE DEHYDROGENASE

Chain B:



• Molecule 1: L-LACTATE DEHYDROGENASE

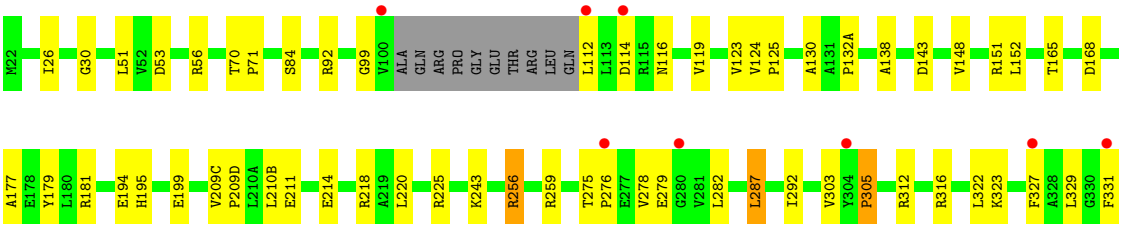
Chain C:



• Molecule 1: L-LACTATE DEHYDROGENASE

Chain D:

3%
78%
18%


M22 I26 G30 L51 V52 D53 R56 T70 P71 S84 R92 G99 V100 ALA GLN ARG PRO GLY GLU THR ARG LEU GLN L112 L113 D114 R115 N116 V119 V123 V124 P125 A130 A131 P132A A138 D143 V148 R151 L152 T165 D168
A177 E178 Y179 L180 R181 E194 H195 E199 V209C P209D L210A L210B E211 E214 R218 A219 L220 R225 K243 R256 R259 T275 P276 E277 V278 E279 G280 V281 L282 L287 I292 V303 Y304 P305 R312 R316 L322 K323 F327 A328 L329 G330 F331

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	151.50Å 142.85Å 59.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.10 45.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (39.16-2.10) 97.8 (45.75-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.204 0.185 , 0.196	Depositor DCC
R_{free} test set	3734 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9824	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, OXM

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	0.40	0/2380	0.62	0/3238
1	B	0.61	3/2280 (0.1%)	0.64	1/3100 (0.0%)
1	C	0.40	0/2367	0.58	1/3220 (0.0%)
1	D	0.35	0/2254	0.55	0/3067
All	All	0.45	3/9281 (0.0%)	0.60	2/12625 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	LEU	C-N	-5.70	1.21	1.34
1	B	127	VAL	C-N	-5.39	1.21	1.34
1	B	328	ALA	CA-CB	-5.28	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	287	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	209(B)	GLY	N-CA-C	-5.33	99.79	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	ARG	Sidechain
1	B	112	LEU	Mainchain
1	B	214	GLU	Peptide
1	B	215	ALA	Peptide
1	C	256	ARG	Sidechain
1	D	92	ARG	Sidechain

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	2324	0	2365	43	0
1	B	2234	0	2273	52	0
1	C	2319	0	2369	56	0
1	D	2212	0	2260	43	0
2	A	6	0	2	0	0
2	B	6	0	2	0	0
2	C	6	0	2	1	0
2	D	6	0	2	0	0
3	A	44	0	24	3	0
3	B	44	0	23	3	0
3	C	44	0	22	4	0
3	D	44	0	24	3	0
4	A	147	0	0	4	0
4	B	136	0	0	4	0
4	C	152	0	0	8	0
4	D	100	0	0	4	0
All	All	9824	0	9368	181	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 10.

All (181) 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:B:113:LEU:HD12	1:B:113:LEU:O	1.37	1.22
1:A:22:MET:CE	1:A:92[B]:ARG:HH11	1.58	1.14
1:A:22:MET:HE1	1:A:92[B]:ARG:HH11	0.99	1.08
1:A:22:MET:HE1	1:A:92[B]:ARG:NH1	1.75	1.01
1:C:316:ARG:HH11	1:C:316:ARG:HG2	1.26	0.99
1:B:113:LEU:HD12	1:B:113:LEU:C	1.85	0.92
1:B:209(C):VAL:HG21	1:C:303:VAL:CG1	2.00	0.90
1:B:215:ALA:HA	1:B:217:GLY:H	1.36	0.89
1:A:22:MET:CE	1:A:92[B]:ARG:NH1	2.32	0.88
1:D:53:ASP:O	1:D:56:ARG:NH1	2.08	0.87
1:B:216:ARG:HD3	4:B:2081:HOH:O	1.75	0.85
1:B:209(C):VAL:HG21	1:C:303:VAL:HG11	1.60	0.83
1:C:306:SER:HA	4:C:2137:HOH:O	1.78	0.81
1:C:126:ARG:HG3	1:C:126:ARG:HH21	1.43	0.81
1:C:179:TYR:CE2	1:C:220:LEU:HD13	2.15	0.80
1:B:256:ARG:NE	1:B:259:ARG:HH21	1.81	0.78
1:C:190:TYR:HE2	1:C:192:LEU:HD11	1.51	0.76
1:A:108:THR:H	1:A:111:GLN:HE21	1.34	0.75
1:B:126:ARG:NH2	1:B:129:GLU:OE1	2.17	0.75
1:C:113:LEU:HD12	1:C:113:LEU:O	1.89	0.73
1:C:316:ARG:HG2	1:C:316:ARG:NH1	2.01	0.72
1:D:194:GLU:HG3	1:D:322:LEU:HD21	1.72	0.71
1:A:156:PRO:HD2	1:A:159:ARG:HG3	1.74	0.69
1:C:179:TYR:CE2	1:C:220:LEU:CD1	2.77	0.67
1:A:223:GLU:HG2	1:A:227:ARG:NH2	2.10	0.66
1:D:316:ARG:HH21	1:D:316:ARG:HG2	1.61	0.66
1:C:190:TYR:CE2	1:C:202:VAL:HG21	2.31	0.66
1:D:148:VAL:O	1:D:152:LEU:HD13	1.95	0.65
1:B:256:ARG:HE	1:B:259:ARG:HH21	1.44	0.65
1:B:26:ILE:HB	1:B:51:LEU:HD23	1.79	0.64
1:D:151:ARG:NE	1:D:331:PHE:O	2.24	0.63
1:B:209(C):VAL:CG2	1:C:303:VAL:HG11	2.29	0.62
1:C:148:VAL:HG22	1:C:331:PHE:CD2	2.34	0.62
1:A:275:THR:HG21	1:A:278:VAL:CG1	2.30	0.61
1:C:241:GLU:HG2	4:C:2103:HOH:O	2.01	0.61
3:C:1332:NAD:H6N	4:C:2109:HOH:O	2.00	0.60
1:B:186:SER:O	1:B:208:VAL:HG13	2.02	0.60
1:D:179:TYR:CZ	1:D:218:ARG:HD3	2.37	0.60
1:C:108:THR:OG1	1:C:111:GLN:HG3	2.02	0.59
1:B:209(B):GLY:HA3	1:C:190:TYR:HE1	1.68	0.59
1:B:24:VAL:HG11	1:B:40:LEU:HD13	1.84	0.59
1:B:209(C):VAL:HG22	1:C:305:PRO:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:NE	1:B:259:ARG:NH2	2.49	0.58
1:C:190:TYR:CD2	1:C:192:LEU:HD21	2.38	0.58
1:A:209(C):VAL:HG21	1:D:303:VAL:CG1	2.33	0.58
1:A:279:GLU:OE1	1:A:312:ARG:CZ	2.51	0.58
1:C:30:GLY:HA3	3:C:1332:NAD:O5B	2.04	0.57
1:B:209(B):GLY:HA3	1:C:190:TYR:CE1	2.38	0.57
1:A:26:ILE:HB	1:A:51:LEU:HD23	1.86	0.56
1:D:256:ARG:NH1	1:D:259:ARG:HH21	2.03	0.56
1:A:138:ALA:O	3:A:1332:NAD:H2N	2.07	0.55
1:C:223:GLU:HB2	4:C:2094:HOH:O	2.07	0.55
1:B:179:TYR:CE2	1:B:220:LEU:CD2	2.90	0.55
1:C:126:ARG:HH21	1:C:126:ARG:CG	2.17	0.55
1:C:210(B):LEU:HD21	1:C:225:ARG:HH21	1.72	0.55
1:A:22:MET:HE3	1:A:92[B]:ARG:HH11	1.61	0.55
1:C:22:MET:HG3	4:C:2009:HOH:O	2.05	0.55
1:C:113:LEU:HD12	1:C:113:LEU:C	2.25	0.55
1:B:111:GLN:O	1:B:115:ARG:HG3	2.07	0.54
1:D:84:SER:HB2	4:D:2011:HOH:O	2.07	0.54
1:B:124:VAL:HB	1:B:125:PRO:HD3	1.90	0.54
1:D:124:VAL:N	1:D:125:PRO:HD2	2.22	0.54
1:D:279:GLU:OE2	1:D:312:ARG:CZ	2.56	0.54
1:B:310:GLU:OE2	4:B:2122:HOH:O	2.18	0.54
1:A:194:GLU:HG3	1:A:322:LEU:HD21	1.91	0.53
1:B:215:ALA:HA	1:B:217:GLY:N	2.16	0.53
1:B:179:TYR:CE2	1:B:220:LEU:HD21	2.44	0.53
1:D:256:ARG:HH11	1:D:259:ARG:HH21	1.56	0.53
1:B:161:VAL:HG22	1:B:298:VAL:HG23	1.91	0.53
1:B:179:TYR:CZ	1:B:220:LEU:HD23	2.43	0.53
1:A:303:VAL:HG11	1:D:209(C):VAL:HG11	1.91	0.53
1:C:56:ARG:HE	1:C:60[A]:GLN:HG3	1.74	0.52
1:A:22:MET:HE3	1:A:92[B]:ARG:NH1	2.20	0.52
1:B:246:THR:OG1	3:B:1332:NAD:H5N	2.10	0.52
1:C:140:ASN:HD22	1:C:142:VAL:H	1.58	0.52
1:B:214:GLU:HG2	1:B:219:ALA:HB1	1.92	0.52
1:C:138:ALA:O	3:C:1332:NAD:H2N	2.10	0.52
1:C:316:ARG:NH1	1:C:316:ARG:CG	2.70	0.52
1:C:190:TYR:CE2	1:C:192:LEU:HD11	2.39	0.51
1:A:316:ARG:HD2	4:A:2139:HOH:O	2.10	0.51
1:C:62:HIS:HE1	4:C:2015:HOH:O	1.93	0.51
1:A:22:MET:CE	1:A:92[A]:ARG:NE	2.74	0.50
1:B:74:HIS:NE2	4:B:2020:HOH:O	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210(B):LEU:HD11	1:D:225:ARG:NH2	2.27	0.49
1:B:239:ILE:CG2	1:B:246:THR:HG22	2.42	0.49
1:C:310:GLU:H	1:C:310:GLU:CD	2.15	0.49
1:A:190:TYR:HE2	1:A:202:VAL:HG21	1.78	0.49
1:D:194:GLU:O	1:D:199:GLU:HB3	2.12	0.49
1:D:292:ILE:HD12	1:D:292:ILE:N	2.26	0.49
1:D:99:GLY:O	3:D:1332:NAD:H8A	2.12	0.49
1:D:275:THR:HG21	1:D:278:VAL:HG22	1.95	0.49
1:C:275:THR:HG21	1:C:278:VAL:CG2	2.43	0.49
1:A:264:ASP:OD1	1:A:266:LYS:NZ	2.41	0.49
1:B:112:LEU:O	1:B:115:ARG:N	2.45	0.49
1:C:140:ASN:HA	1:C:142:VAL:N	2.27	0.49
1:C:277:GLU:OE2	1:C:280:GLY:N	2.37	0.49
1:B:54:LEU:HG	3:B:1332:NAD:C6A	2.44	0.48
1:D:70:THR:N	1:D:71:PRO:CD	2.76	0.48
1:D:165:THR:HA	1:D:168:ASP:OD2	2.14	0.48
1:C:62:HIS:CD2	1:D:243:LYS:NZ	2.81	0.48
1:C:179:TYR:CZ	1:C:220:LEU:CD1	2.96	0.48
1:A:185:GLN:HB3	4:A:2079:HOH:O	2.14	0.48
1:A:209(C):VAL:HG22	1:D:305:PRO:HA	1.96	0.48
2:C:501:OXM:C1	3:C:1332:NAD:C4N	2.92	0.48
1:C:324:GLU:HA	1:C:324:GLU:OE1	2.13	0.48
1:D:116:ASN:ND2	4:D:2032:HOH:O	2.46	0.48
1:A:165:THR:HA	1:A:168:ASP:OD2	2.14	0.47
1:B:213:ALA:HB1	1:B:218:ARG:O	2.14	0.47
1:D:327:PHE:C	1:D:329:LEU:H	2.16	0.47
1:A:22:MET:HE2	1:A:92[A]:ARG:HG3	1.96	0.47
1:B:310:GLU:HG3	4:B:2123:HOH:O	2.15	0.47
1:A:223:GLU:HG2	1:A:227:ARG:HH22	1.77	0.47
1:A:279:GLU:OE1	1:A:279:GLU:HA	2.15	0.47
1:A:22:MET:HE1	1:A:92[B]:ARG:HD3	1.97	0.46
1:B:209(D):PRO:O	1:B:210(A):LEU:C	2.53	0.46
1:A:22:MET:CE	1:A:92[A]:ARG:HG3	2.46	0.46
1:C:202:VAL:HG12	1:C:202:VAL:O	2.15	0.46
1:B:194:GLU:O	1:B:199:GLU:HB3	2.15	0.46
1:A:124:VAL:HB	1:A:125:PRO:HD3	1.97	0.45
1:B:190:TYR:CE2	1:B:192:LEU:HD21	2.51	0.45
1:A:250:ILE:HD13	3:A:1332:NAD:N7N	2.31	0.45
1:A:92[B]:ARG:NE	4:A:2035:HOH:O	2.14	0.45
1:C:62:HIS:HD2	1:D:243:LYS:NZ	2.15	0.45
1:D:119:VAL:O	1:D:123:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210(B):LEU:O	1:D:214:GLU:HG3	2.18	0.44
1:B:214:GLU:HG2	1:B:219:ALA:CB	2.48	0.44
1:B:52:VAL:HG22	1:B:83:GLY:O	2.17	0.44
1:C:62:HIS:HD2	1:D:243:LYS:HZ3	1.66	0.44
1:D:26:ILE:HB	1:D:51:LEU:HD23	1.99	0.44
1:C:287:LEU:C	1:C:287:LEU:HD23	2.38	0.44
1:D:210(B):LEU:CD1	4:D:2056:HOH:O	2.65	0.43
1:B:70:THR:N	1:B:71:PRO:CD	2.80	0.43
1:C:220:LEU:HD12	1:C:220:LEU:HA	1.75	0.43
1:A:70:THR:N	1:A:71:PRO:CD	2.82	0.43
1:B:165:THR:HA	1:B:168:ASP:OD2	2.18	0.43
1:A:140:ASN:HD22	1:A:142:VAL:H	1.64	0.43
1:D:143:ASP:OD2	1:D:194:GLU:HA	2.19	0.43
1:C:151:ARG:NE	1:C:331:PHE:OXT	2.43	0.43
1:A:30:GLY:HA3	3:A:1332:NAD:O5B	2.19	0.42
1:C:105:PRO:HB3	1:C:241:GLU:OE2	2.19	0.42
1:D:282:LEU:O	1:D:323:LYS:HE2	2.19	0.42
1:B:121:ALA:HA	1:B:152:LEU:HD13	2.00	0.42
1:B:210(B):LEU:HA	1:B:210(B):LEU:HD12	1.64	0.42
1:C:306:SER:O	1:C:307:LEU:HD23	2.19	0.42
1:A:68:HIS:CG	1:B:171:ARG:HG2	2.54	0.42
1:D:56:ARG:NH2	4:D:2011:HOH:O	2.52	0.42
1:A:98:ALA:O	1:A:139[A]:THR:CG2	2.67	0.42
1:B:113:LEU:O	1:B:113:LEU:CD1	2.32	0.42
1:B:214:GLU:HA	1:B:219:ALA:HA	2.01	0.42
1:C:194:GLU:O	1:C:199:GLU:HB3	2.20	0.42
1:D:275:THR:HA	1:D:276:PRO:HD3	1.94	0.42
1:C:177:ALA:HB1	1:C:182:VAL:O	2.20	0.42
1:D:287:LEU:HB3	1:D:322:LEU:CD1	2.49	0.42
1:A:62:HIS:CE1	1:B:243:LYS:HD2	2.55	0.42
1:B:115:ARG:O	1:B:119:VAL:HG23	2.19	0.42
1:C:22:MET:HE3	1:C:22:MET:HB3	1.77	0.41
1:C:310:GLU:CD	1:C:310:GLU:N	2.74	0.41
1:A:92[B]:ARG:HD2	4:A:2036:HOH:O	2.20	0.41
1:D:30:GLY:HA3	3:D:1332:NAD:O5B	2.20	0.41
1:D:179:TYR:CE1	1:D:218:ARG:HD3	2.56	0.41
1:B:138:ALA:O	3:B:1332:NAD:H2N	2.20	0.41
1:D:138:ALA:O	3:D:1332:NAD:H2N	2.21	0.41
1:D:220:LEU:HD23	1:D:220:LEU:HA	1.89	0.41
1:A:190:TYR:CE2	1:A:202:VAL:HG21	2.55	0.41
1:B:56:ARG:HA	1:B:56:ARG:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ALA:O	1:D:181:ARG:N	2.54	0.41
1:D:209(D):PRO:HB2	1:D:211:GLU:HG2	2.03	0.41
1:C:179:TYR:CZ	1:C:218:ARG:HD2	2.56	0.41
1:D:130:ALA:O	1:D:132(A):PRO:HD3	2.21	0.41
1:A:194:GLU:O	1:A:199:GLU:HB3	2.20	0.41
1:A:278:VAL:O	1:A:278:VAL:HG23	2.21	0.41
1:B:24:VAL:CG1	1:B:49:VAL:HG22	2.51	0.41
1:B:209(C):VAL:HG21	1:C:303:VAL:HG12	1.97	0.41
1:C:172:PHE:CE1	1:C:176:LEU:HD11	2.56	0.41
1:C:22:MET:N	4:C:2001:HOH:O	2.54	0.41
1:D:316:ARG:HG2	1:D:316:ARG:NH2	2.34	0.41
1:B:287:LEU:O	1:B:291:ARG:NH1	2.53	0.40
1:A:275:THR:HG21	1:A:278:VAL:HG11	2.00	0.40
1:C:223:GLU:CB	4:C:2094:HOH:O	2.68	0.40
1:A:98:ALA:O	1:A:139[A]:THR:HG21	2.22	0.40
1:C:210(B):LEU:HD21	1:C:225:ARG:NH2	2.35	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	312/310 (101%)	302 (97%)	10 (3%)	0	100	100
1	B	297/310 (96%)	289 (97%)	8 (3%)	0	100	100
1	C	310/310 (100%)	304 (98%)	6 (2%)	0	100	100
1	D	297/310 (96%)	288 (97%)	7 (2%)	2 (1%)	22	18
All	All	1216/1240 (98%)	1183 (97%)	31 (2%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	195	HIS
1	D	305	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	233/232 (100%)	226 (97%)	7 (3%)	41	44
1	B	223/232 (96%)	219 (98%)	4 (2%)	59	65
1	C	233/232 (100%)	228 (98%)	5 (2%)	53	59
1	D	218/232 (94%)	214 (98%)	4 (2%)	59	65
All	All	907/928 (98%)	887 (98%)	20 (2%)	52	57

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	TYR
1	A	216	ARG
1	A	218	ARG
1	A	241	GLU
1	A	246	THR
1	A	287	LEU
1	A	312	ARG
1	B	113	LEU
1	B	136	LEU
1	B	210(B)	LEU
1	B	216	ARG
1	C	22	MET
1	C	92	ARG
1	C	220	LEU
1	C	246	THR
1	C	287	LEU
1	D	112	LEU
1	D	114	ASP
1	D	256	ARG
1	D	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	111	GLN
1	A	140	ASN
1	B	62	HIS
1	B	118	GLN
1	B	140	ASN
1	C	62	HIS
1	C	140	ASN
1	D	140	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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	C	1332	-	42,48,48	2.54	22 (52%)	50,73,73	2.31	16 (32%)
3	NAD	D	1332	-	42,48,48	2.63	16 (38%)	50,73,73	2.27	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OXM	A	501	-	5,5,5	2.38	2 (40%)	4,6,6	2.42	2 (50%)
2	OXM	B	501	-	5,5,5	1.17	0	4,6,6	1.26	0
3	NAD	A	1332	-	42,48,48	2.83	17 (40%)	50,73,73	2.49	19 (38%)
3	NAD	B	1332	-	42,48,48	2.95	18 (42%)	50,73,73	2.51	16 (32%)
2	OXM	C	501	-	5,5,5	1.00	0	4,6,6	1.08	0
2	OXM	D	501	-	5,5,5	0.94	0	4,6,6	2.01	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	1332	-	-	5/26/62/62	0/5/5/5
3	NAD	D	1332	-	1/1/11/11	4/26/62/62	0/5/5/5
2	OXM	A	501	-	-	3/3/4/4	-
2	OXM	B	501	-	-	3/3/4/4	-
3	NAD	A	1332	-	-	5/26/62/62	0/5/5/5
3	NAD	B	1332	-	-	5/26/62/62	0/5/5/5
2	OXM	C	501	-	-	3/3/4/4	-
2	OXM	D	501	-	-	3/3/4/4	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1332	NAD	O4D-C1D	-9.04	1.28	1.41
3	A	1332	NAD	PA-O5B	-6.17	1.34	1.59
3	D	1332	NAD	O7N-C7N	5.98	1.35	1.24
3	D	1332	NAD	C2N-N1N	5.72	1.41	1.35
3	B	1332	NAD	O4B-C1B	-5.61	1.33	1.41
3	A	1332	NAD	PA-O2A	-5.60	1.29	1.55
3	A	1332	NAD	PN-O2N	-5.58	1.29	1.55
3	A	1332	NAD	O7N-C7N	5.40	1.34	1.24
3	C	1332	NAD	C2B-C1B	-5.23	1.45	1.53
3	A	1332	NAD	PA-O1A	-5.19	1.32	1.50
3	D	1332	NAD	PN-O2N	-5.05	1.31	1.55
3	C	1332	NAD	O5D-C5D	-5.01	1.25	1.44
3	B	1332	NAD	PA-O2A	-5.00	1.31	1.55
3	C	1332	NAD	PN-O5D	-4.98	1.39	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1332	NAD	PN-O2N	-4.57	1.33	1.55
3	D	1332	NAD	O5D-C5D	-4.57	1.27	1.44
3	A	1332	NAD	PN-O5D	-4.55	1.40	1.59
3	B	1332	NAD	O7N-C7N	4.52	1.32	1.24
3	D	1332	NAD	PN-O1N	-4.49	1.35	1.50
3	B	1332	NAD	PA-O1A	-4.49	1.35	1.50
3	A	1332	NAD	O3D-C3D	-4.47	1.32	1.43
3	A	1332	NAD	O4D-C1D	-4.43	1.34	1.41
3	D	1332	NAD	PN-O5D	-4.43	1.41	1.59
3	B	1332	NAD	C7N-N7N	-4.33	1.24	1.33
3	C	1332	NAD	PN-O2N	-4.21	1.35	1.55
3	D	1332	NAD	O5B-C5B	-4.16	1.28	1.44
3	D	1332	NAD	C2B-C1B	-4.10	1.47	1.53
3	D	1332	NAD	PA-O2A	-4.09	1.36	1.55
2	A	501	OXM	O3-C2	-4.07	1.18	1.30
3	B	1332	NAD	C8A-N7A	-3.89	1.27	1.34
3	D	1332	NAD	PA-O5B	-3.77	1.44	1.59
3	C	1332	NAD	O7N-C7N	3.75	1.31	1.24
3	C	1332	NAD	O3D-C3D	-3.69	1.34	1.43
3	C	1332	NAD	PA-O1A	-3.68	1.37	1.50
3	B	1332	NAD	O4B-C4B	-3.68	1.36	1.45
3	D	1332	NAD	C8A-N7A	-3.67	1.28	1.34
3	B	1332	NAD	C2B-C1B	-3.61	1.48	1.53
3	C	1332	NAD	O4B-C1B	-3.57	1.36	1.41
3	A	1332	NAD	O5B-C5B	-3.49	1.31	1.44
3	A	1332	NAD	C8A-N7A	-3.48	1.28	1.34
3	B	1332	NAD	O5B-C5B	-3.45	1.31	1.44
3	B	1332	NAD	O3D-C3D	-3.38	1.35	1.43
3	C	1332	NAD	PA-O2A	-3.35	1.39	1.55
3	C	1332	NAD	O5B-C5B	-3.33	1.31	1.44
3	B	1332	NAD	C5A-N7A	-3.28	1.27	1.39
3	A	1332	NAD	PN-O1N	-3.25	1.39	1.50
2	A	501	OXM	C1-C2	-3.15	1.51	1.55
3	A	1332	NAD	C5A-N7A	-3.15	1.28	1.39
3	C	1332	NAD	PN-O1N	-3.13	1.39	1.50
3	B	1332	NAD	C5D-C4D	-3.10	1.42	1.51
3	A	1332	NAD	C7N-N7N	-3.06	1.27	1.33
3	C	1332	NAD	O4B-C4B	-3.05	1.38	1.45
3	D	1332	NAD	PA-O1A	-3.01	1.40	1.50
3	B	1332	NAD	O4D-C4D	-2.95	1.38	1.45
3	C	1332	NAD	C5A-N7A	-2.91	1.29	1.39
3	D	1332	NAD	C5A-N7A	-2.82	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1332	NAD	C2N-N1N	2.81	1.38	1.35
3	D	1332	NAD	C5B-C4B	-2.76	1.43	1.51
3	C	1332	NAD	O3B-C3B	-2.74	1.36	1.43
3	B	1332	NAD	O3B-C3B	-2.59	1.36	1.43
3	A	1332	NAD	O4B-C1B	-2.58	1.37	1.41
3	A	1332	NAD	C2B-C1B	-2.57	1.49	1.53
3	B	1332	NAD	PN-O1N	-2.57	1.41	1.50
3	D	1332	NAD	O3D-C3D	-2.53	1.37	1.43
3	B	1332	NAD	PN-O5D	-2.51	1.49	1.59
3	C	1332	NAD	C6A-C5A	2.45	1.52	1.43
3	C	1332	NAD	O2B-C2B	-2.39	1.37	1.43
3	C	1332	NAD	C6A-N6A	2.34	1.42	1.34
3	D	1332	NAD	O4B-C4B	-2.24	1.40	1.45
3	A	1332	NAD	O2D-C2D	-2.23	1.37	1.43
3	C	1332	NAD	C8A-N7A	-2.23	1.30	1.34
3	C	1332	NAD	C3D-C4D	2.21	1.58	1.53
3	C	1332	NAD	C2A-N3A	2.19	1.35	1.32
3	C	1332	NAD	C7N-N7N	-2.12	1.28	1.33
3	C	1332	NAD	C2B-C3B	-2.10	1.47	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1332	NAD	O4D-C1D-C2D	-7.86	95.43	106.93
3	C	1332	NAD	O4B-C4B-C5B	6.67	131.33	109.37
3	B	1332	NAD	O4D-C1D-C2D	-6.58	97.30	106.93
3	A	1332	NAD	O4B-C4B-C5B	6.47	130.68	109.37
3	C	1332	NAD	O4B-C1B-C2B	-6.43	97.52	106.93
3	B	1332	NAD	C2D-C3D-C4D	-6.32	90.36	102.64
3	B	1332	NAD	O4B-C4B-C5B	6.00	129.13	109.37
3	D	1332	NAD	O4B-C4B-C5B	5.97	129.03	109.37
3	D	1332	NAD	N3A-C2A-N1A	-5.80	119.61	128.68
3	B	1332	NAD	O4D-C4D-C5D	5.69	128.11	109.37
3	D	1332	NAD	O4D-C4D-C3D	-5.27	94.69	105.11
3	A	1332	NAD	C6N-N1N-C2N	-5.24	117.20	121.97
3	B	1332	NAD	O4B-C1B-C2B	-4.93	99.72	106.93
3	C	1332	NAD	C3D-C2D-C1D	-4.77	93.80	100.98
3	C	1332	NAD	O4D-C4D-C3D	-4.76	95.70	105.11
3	C	1332	NAD	N3A-C2A-N1A	-4.69	121.35	128.68
3	D	1332	NAD	C3D-C2D-C1D	-4.39	94.36	100.98
3	C	1332	NAD	O5D-C5D-C4D	4.27	123.68	108.99
3	B	1332	NAD	C6N-N1N-C2N	-4.09	118.24	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1332	NAD	O5D-C5D-C4D	-3.92	95.49	108.99
2	A	501	OXM	O3-C2-C1	3.92	122.90	113.84
3	D	1332	NAD	O5D-C5D-C4D	3.86	122.28	108.99
3	A	1332	NAD	O5B-C5B-C4B	3.69	121.69	108.99
3	A	1332	NAD	C3N-C7N-N7N	-3.61	113.42	117.75
3	A	1332	NAD	O4D-C4D-C5D	-3.54	97.73	109.37
3	A	1332	NAD	C3N-C2N-N1N	3.52	123.87	120.43
3	A	1332	NAD	C3D-C2D-C1D	-3.48	95.74	100.98
3	D	1332	NAD	C2B-C3B-C4B	-3.36	96.12	102.64
3	B	1332	NAD	C1B-N9A-C4A	3.30	132.44	126.64
3	A	1332	NAD	N3A-C2A-N1A	-3.26	123.58	128.68
3	A	1332	NAD	O4D-C4D-C3D	-3.19	98.81	105.11
3	A	1332	NAD	C5N-C4N-C3N	-3.16	116.60	120.34
3	B	1332	NAD	N3A-C2A-N1A	-3.15	123.75	128.68
3	B	1332	NAD	O4D-C4D-C3D	3.14	111.33	105.11
3	A	1332	NAD	O5D-C5D-C4D	3.10	119.67	108.99
2	D	501	OXM	O2-C2-C1	-3.05	115.27	122.06
3	C	1332	NAD	C1B-N9A-C4A	3.03	131.96	126.64
3	C	1332	NAD	O5B-C5B-C4B	2.99	119.28	108.99
3	B	1332	NAD	C2N-C3N-C4N	2.98	121.64	118.26
3	A	1332	NAD	C5D-C4D-C3D	2.98	126.35	115.18
3	D	1332	NAD	C1B-N9A-C4A	2.87	131.68	126.64
3	D	1332	NAD	O4B-C1B-C2B	-2.85	102.76	106.93
3	D	1332	NAD	O5B-PA-O1A	-2.79	98.15	109.07
3	D	1332	NAD	O2D-C2D-C1D	-2.69	100.91	110.85
3	A	1332	NAD	C2B-C3B-C4B	-2.69	97.42	102.64
3	C	1332	NAD	O7N-C7N-C3N	2.67	122.83	119.63
3	C	1332	NAD	C5A-C6A-N6A	2.66	124.40	120.35
3	B	1332	NAD	O5B-C5B-C4B	2.66	118.14	108.99
3	A	1332	NAD	O3B-C3B-C4B	2.61	118.59	111.05
3	D	1332	NAD	O4D-C4D-C5D	2.60	117.91	109.37
3	D	1332	NAD	O5B-C5B-C4B	2.58	117.88	108.99
3	A	1332	NAD	C5A-C6A-N6A	2.55	124.23	120.35
3	D	1332	NAD	C6N-C5N-C4N	2.55	123.15	119.44
3	A	1332	NAD	C1B-N9A-C4A	2.54	131.09	126.64
3	C	1332	NAD	C6N-N1N-C2N	-2.51	119.69	121.97
3	A	1332	NAD	O4B-C1B-C2B	-2.49	103.29	106.93
3	B	1332	NAD	C2B-C3B-C4B	-2.47	97.85	102.64
3	D	1332	NAD	O3D-C3D-C2D	2.46	119.77	111.82
3	B	1332	NAD	PN-O5D-C5D	2.45	136.03	121.68
3	C	1332	NAD	O7N-C7N-N7N	-2.40	119.17	122.58
3	C	1332	NAD	C2B-C3B-C4B	-2.37	98.04	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1332	NAD	O2D-C2D-C1D	2.37	119.61	110.85
3	D	1332	NAD	O3B-C3B-C4B	2.37	117.89	111.05
3	D	1332	NAD	C2N-N1N-C1D	2.33	124.32	119.14
3	C	1332	NAD	O3D-C3D-C4D	2.29	117.67	111.05
2	A	501	OXM	O2-C2-C1	-2.26	117.02	122.06
2	D	501	OXM	O3-C2-C1	2.25	119.05	113.84
3	A	1332	NAD	C6N-C5N-C4N	2.07	122.45	119.44
3	D	1332	NAD	C6N-N1N-C2N	-2.07	120.09	121.97
3	C	1332	NAD	C5A-C6A-N1A	-2.02	115.76	120.35
3	B	1332	NAD	O3B-C3B-C4B	2.02	116.90	111.05
3	C	1332	NAD	C2N-N1N-C1D	2.00	123.60	119.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1332	NAD	C4B

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	OXM	N1-C1-C2-O2
2	A	501	OXM	N1-C1-C2-O3
2	A	501	OXM	O1-C1-C2-O2
2	B	501	OXM	N1-C1-C2-O2
2	B	501	OXM	N1-C1-C2-O3
2	B	501	OXM	O1-C1-C2-O2
2	C	501	OXM	N1-C1-C2-O2
2	C	501	OXM	N1-C1-C2-O3
2	C	501	OXM	O1-C1-C2-O2
2	D	501	OXM	N1-C1-C2-O2
2	D	501	OXM	N1-C1-C2-O3
2	D	501	OXM	O1-C1-C2-O2
3	A	1332	NAD	O4B-C4B-C5B-O5B
3	A	1332	NAD	O4D-C1D-N1N-C2N
3	A	1332	NAD	O4D-C1D-N1N-C6N
3	A	1332	NAD	C2D-C1D-N1N-C2N
3	A	1332	NAD	C2D-C1D-N1N-C6N
3	B	1332	NAD	O4D-C1D-N1N-C6N
3	B	1332	NAD	C2D-C1D-N1N-C2N
3	C	1332	NAD	O4D-C1D-N1N-C2N
3	C	1332	NAD	O4D-C1D-N1N-C6N
3	C	1332	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	D	1332	NAD	O4D-C1D-N1N-C2N
3	D	1332	NAD	C2D-C1D-N1N-C2N
3	D	1332	NAD	C2D-C1D-N1N-C6N
3	C	1332	NAD	O4B-C4B-C5B-O5B
3	D	1332	NAD	O4B-C4B-C5B-O5B
3	B	1332	NAD	C3D-C4D-C5D-O5D
3	B	1332	NAD	O4B-C4B-C5B-O5B
3	B	1332	NAD	C2D-C1D-N1N-C6N
3	C	1332	NAD	C2D-C1D-N1N-C2N

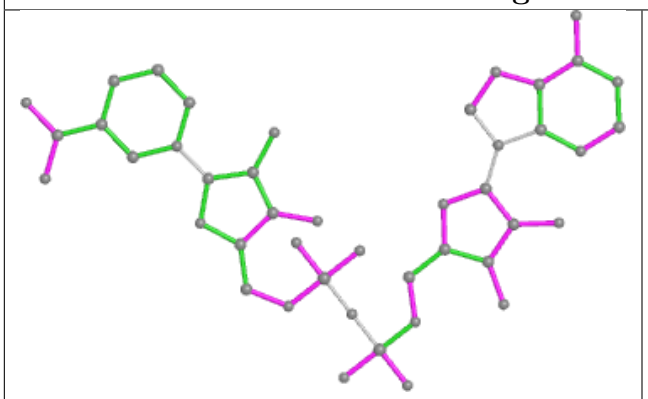
There are no ring outliers.

5 monomers are involved in 13 short contacts:

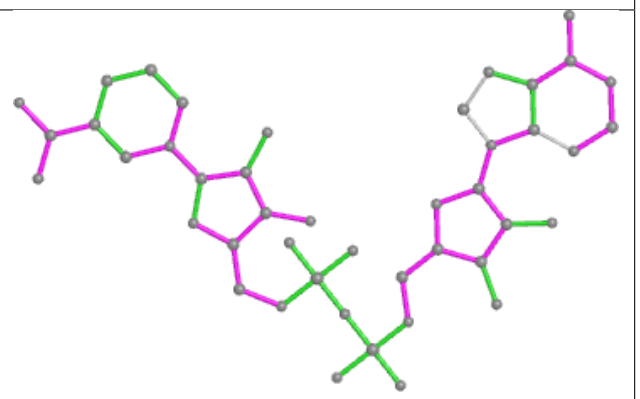
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1332	NAD	4	0
3	D	1332	NAD	3	0
3	A	1332	NAD	3	0
3	B	1332	NAD	3	0
2	C	501	OXM	1	0

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.

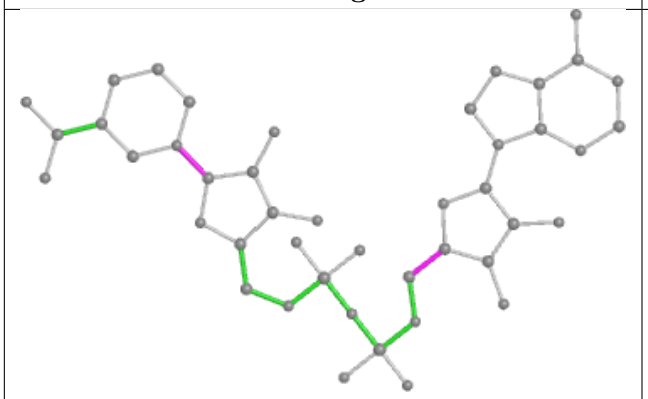
Ligand NAD C 1332



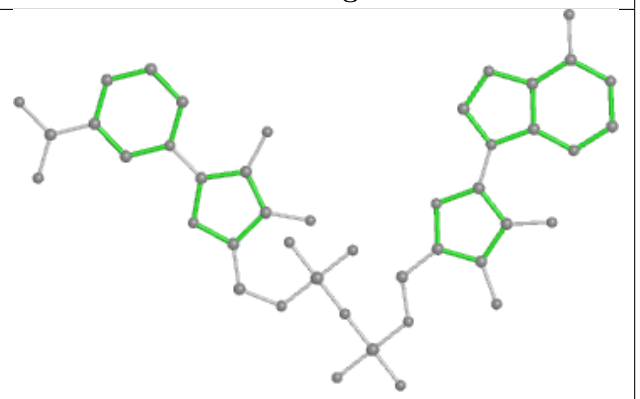
Bond lengths



Bond angles

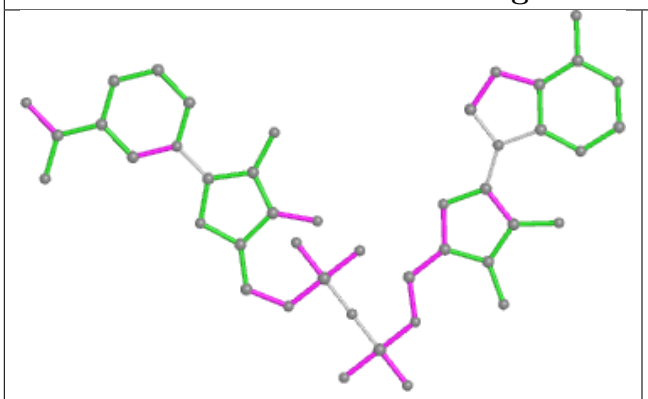


Torsions

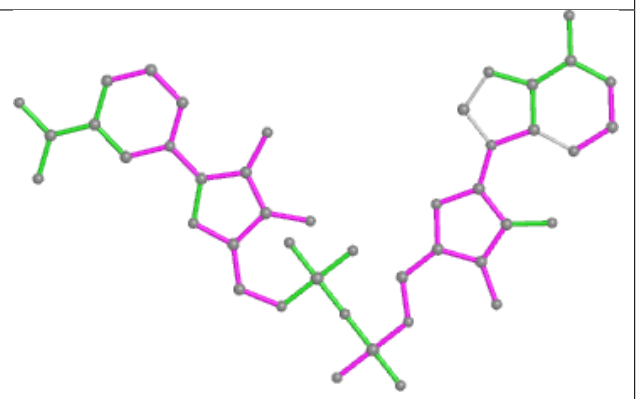


Rings

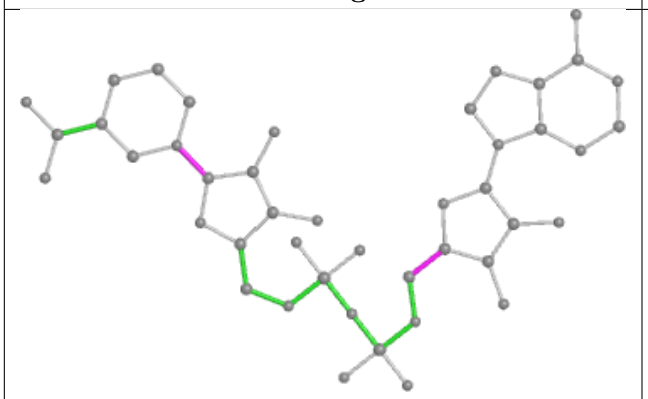
Ligand NAD D 1332



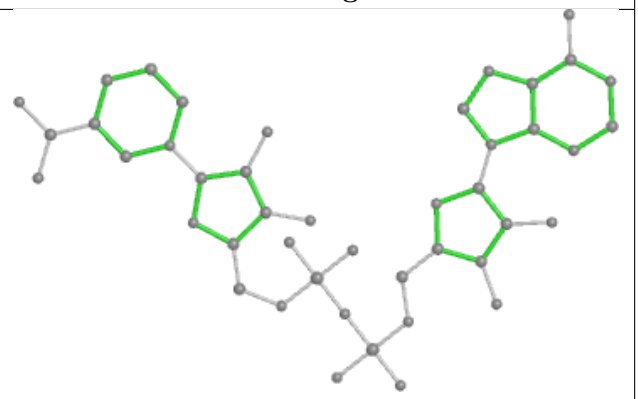
Bond lengths



Bond angles

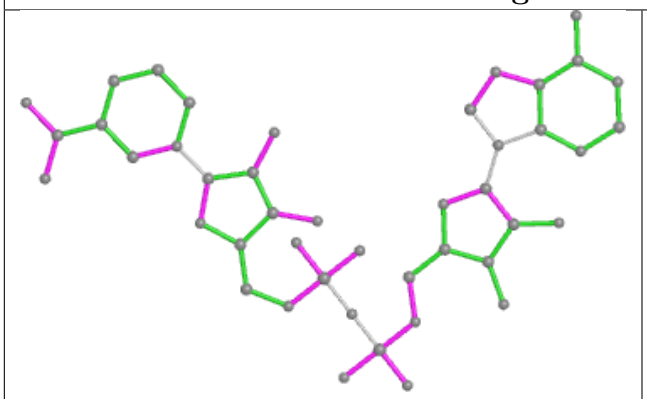


Torsions

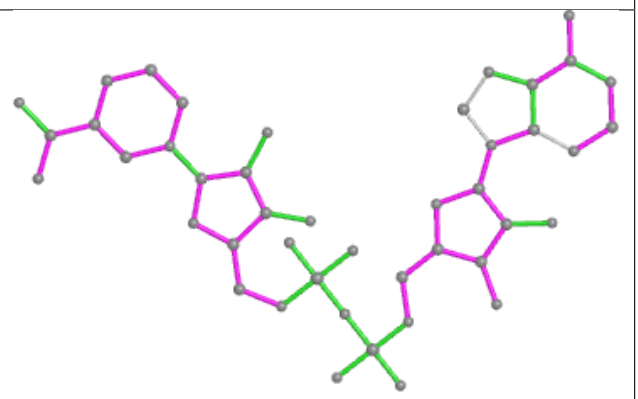


Rings

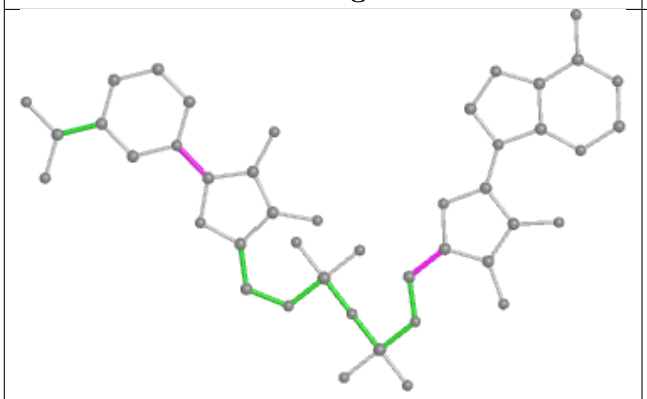
Ligand NAD A 1332



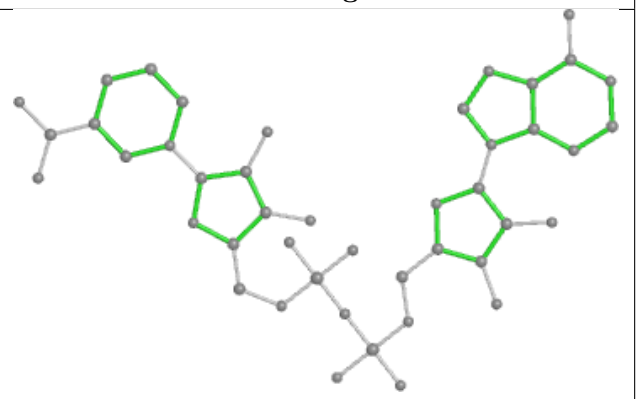
Bond lengths



Bond angles

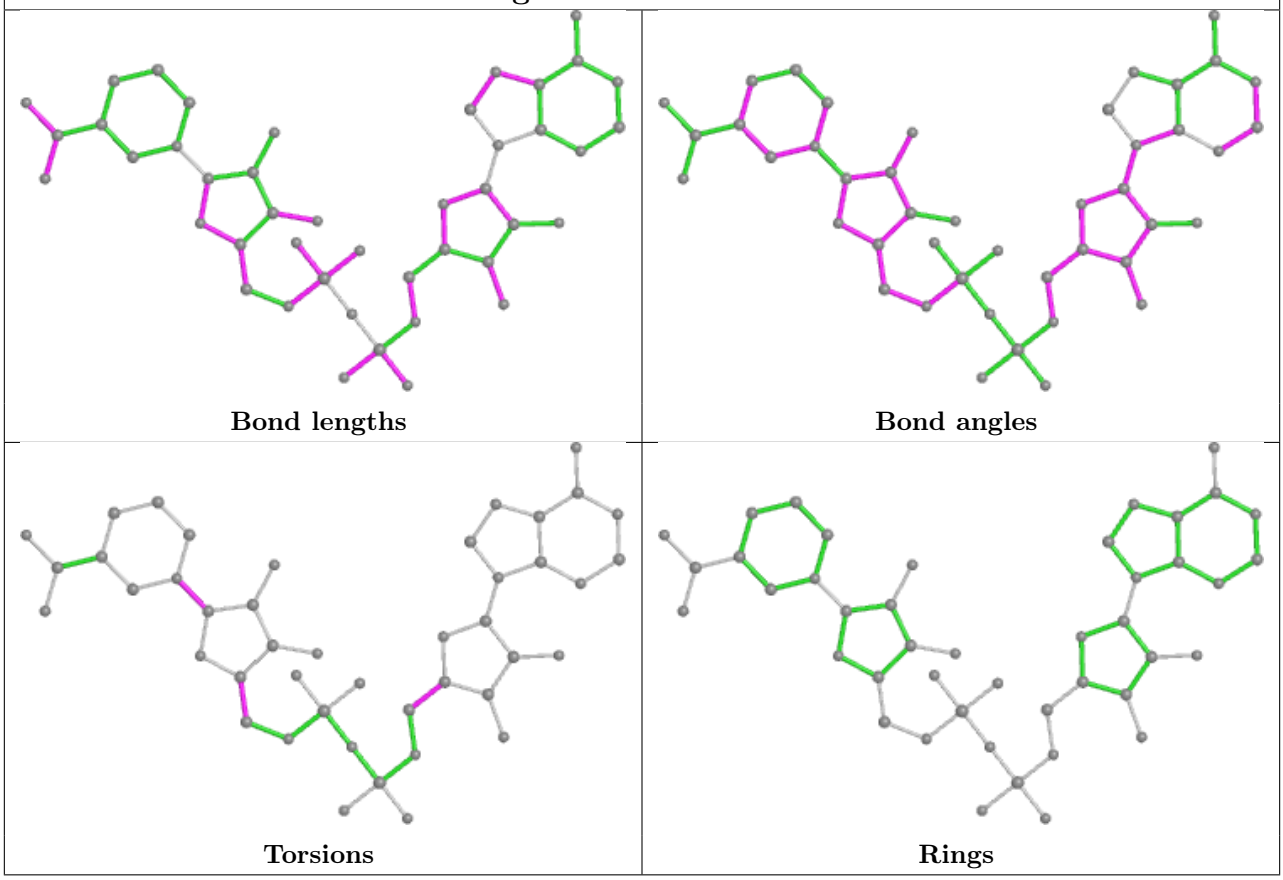


Torsions



Rings

Ligand NAD B 1332



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	310/310 (100%)	-0.13	4 (1%)	77	80	10, 22, 36, 46	15 (4%)
1	B	299/310 (96%)	-0.13	13 (4%)	35	41	12, 22, 40, 58	21 (7%)
1	C	310/310 (100%)	-0.30	1 (0%)	94	94	12, 21, 40, 51	12 (3%)
1	D	300/310 (96%)	-0.01	8 (2%)	54	60	16, 27, 44, 61	14 (4%)
All	All	1219/1240 (98%)	-0.14	26 (2%)	63	68	10, 22, 41, 61	62 (5%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	VAL	5.2
1	B	112	LEU	4.3
1	D	327	PHE	3.6
1	D	112	LEU	3.4
1	D	331	PHE	3.3
1	B	209(A)	GLY	3.1
1	C	190	TYR	3.1
1	B	331	PHE	3.1
1	B	209(C)	VAL	2.9
1	B	209(B)	GLY	2.9
1	A	106	GLY	2.8
1	D	304	TYR	2.7
1	A	43	LEU	2.5
1	D	114	ASP	2.4
1	D	276	PRO	2.4
1	B	214	GLU	2.4
1	B	42	LEU	2.3
1	A	220	LEU	2.2
1	D	280	GLY	2.2
1	B	218	ARG	2.2
1	B	111	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	219	ALA	2.1
1	B	209(D)	PRO	2.1
1	A	42	LEU	2.0
1	B	223	GLU	2.0
1	B	73	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

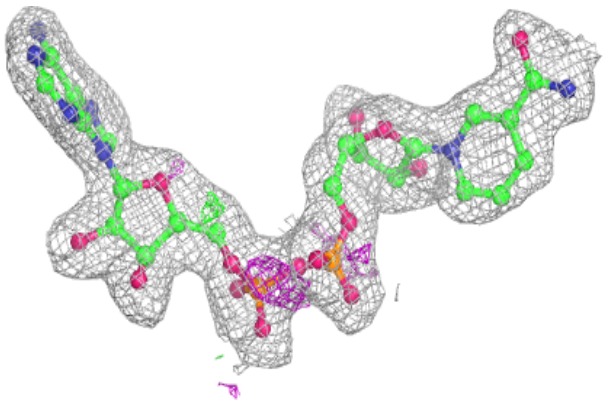
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

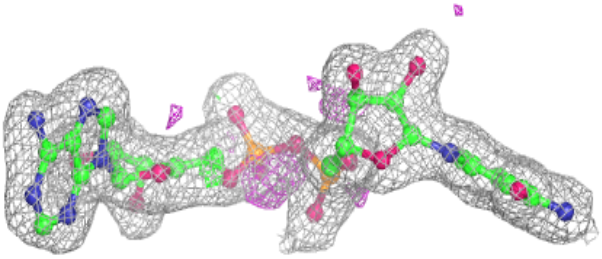
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OXM	A	501	6/6	0.92	0.14	26,27,28,28	0
2	OXM	C	501	6/6	0.94	0.18	25,27,29,30	0
2	OXM	B	501	6/6	0.95	0.11	25,27,28,28	0
2	OXM	D	501	6/6	0.95	0.13	24,27,29,29	0
3	NAD	D	1332	44/44	0.95	0.10	19,27,29,32	0
3	NAD	C	1332	44/44	0.96	0.10	19,25,28,30	0
3	NAD	B	1332	44/44	0.96	0.10	17,24,26,28	0
3	NAD	A	1332	44/44	0.97	0.09	12,18,23,24	0

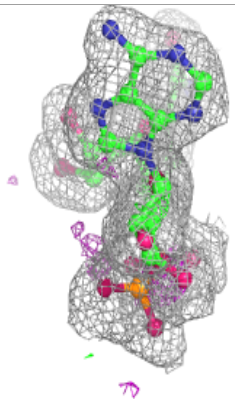
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 1332:

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

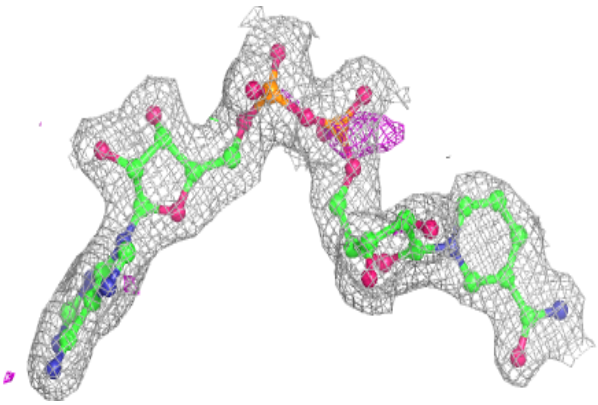


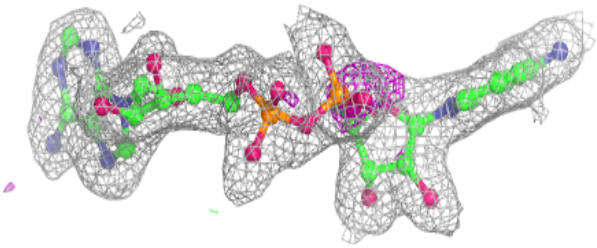


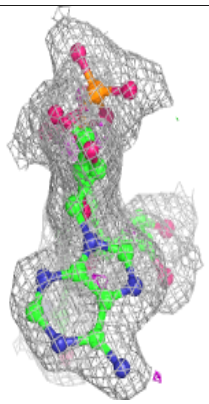


Electron density around NAD C 1332:

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

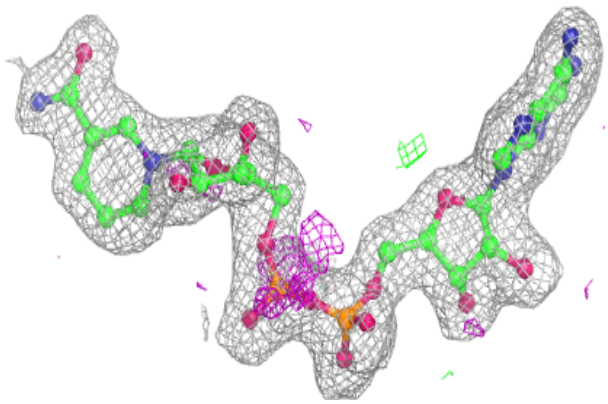


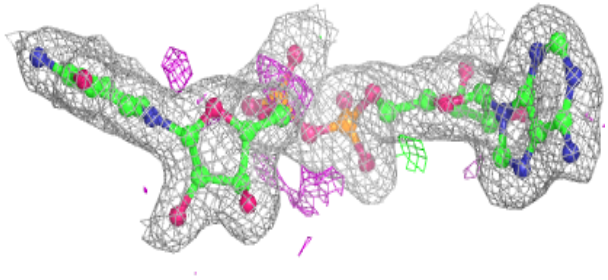


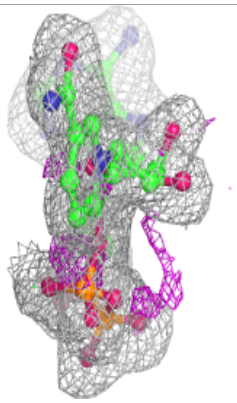


Electron density around NAD B 1332:

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

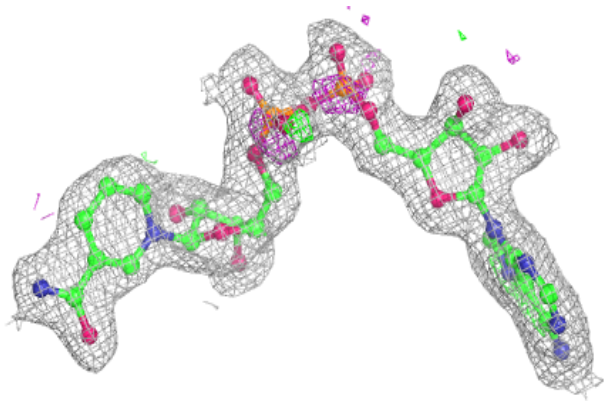


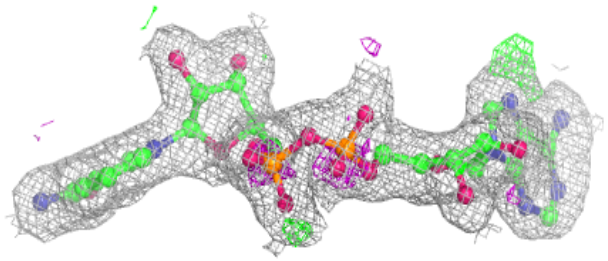


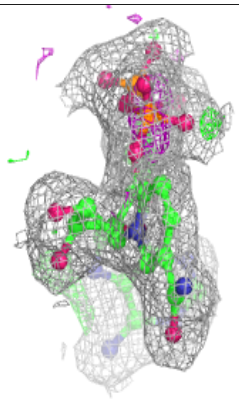


Electron density around NAD A 1332:

$2mF_o$-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.