



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:06 AM GMT

PDB ID : 3DBV
Title : GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE MUTANT
WITH LEU 33 REPLACED BY THR, THR 34 REPLACED BY GLY, ASP
36 REPLACED BY GLY, LEU 187 REPLACED BY ALA, AND PRO 188
REPLACED BY SER COMPLEXED WITH NAD⁺
Authors : Didierjean, C.; Rahuel-Clermont, S.; Vitoux, B.; Dideberg, O.; Branlant, G.;
Aubry, A.
Deposited on : 1997-01-06
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

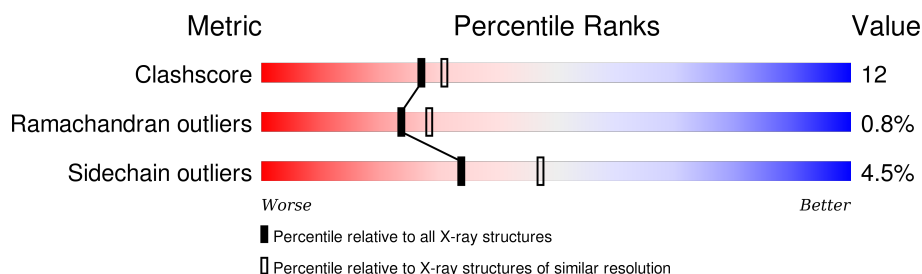
1 Overall quality at a glance

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))
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	O	334	
1	P	334	
1	Q	334	
1	R	334	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10559 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2513	1571	445	488	9			
1	P	334	Total	C	N	O	S	0	0	0
			2513	1571	445	488	9			
1	Q	334	Total	C	N	O	S	0	0	0
			2513	1571	445	488	9			
1	R	334	Total	C	N	O	S	0	0	0
			2513	1571	445	488	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	33	THR	LEU	ENGINEERED	UNP P00362
O	34	GLY	THR	ENGINEERED	UNP P00362
O	36	GLY	ASP	ENGINEERED	UNP P00362
O	187	ALA	LEU	ENGINEERED	UNP P00362
O	188	SER	PRO	ENGINEERED	UNP P00362
P	33	THR	LEU	ENGINEERED	UNP P00362
P	34	GLY	THR	ENGINEERED	UNP P00362
P	36	GLY	ASP	ENGINEERED	UNP P00362
P	187	ALA	LEU	ENGINEERED	UNP P00362
P	188	SER	PRO	ENGINEERED	UNP P00362
Q	33	THR	LEU	ENGINEERED	UNP P00362
Q	34	GLY	THR	ENGINEERED	UNP P00362
Q	36	GLY	ASP	ENGINEERED	UNP P00362
Q	187	ALA	LEU	ENGINEERED	UNP P00362
Q	188	SER	PRO	ENGINEERED	UNP P00362
R	33	THR	LEU	ENGINEERED	UNP P00362
R	34	GLY	THR	ENGINEERED	UNP P00362
R	36	GLY	ASP	ENGINEERED	UNP P00362
R	187	ALA	LEU	ENGINEERED	UNP P00362
R	188	SER	PRO	ENGINEERED	UNP P00362

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

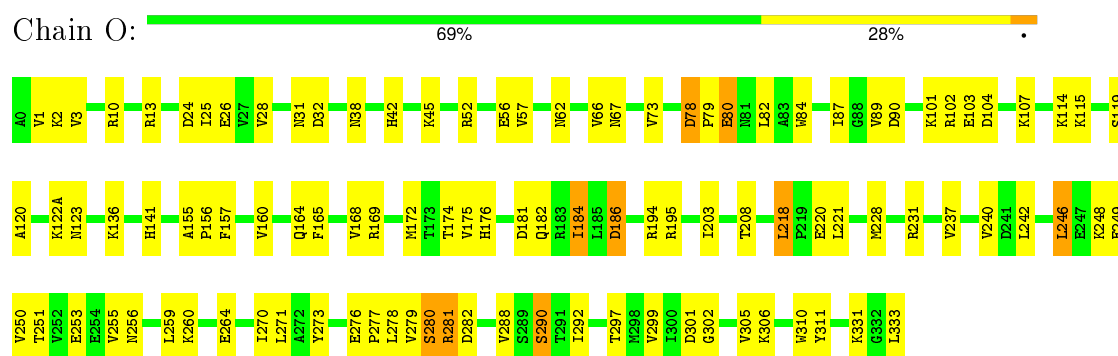
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	81	Total	O	0	0
			81	81		
4	P	77	Total	O	0	0
			77	77		
4	Q	66	Total	O	0	0
			66	66		
4	R	67	Total	O	0	0
			67	67		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

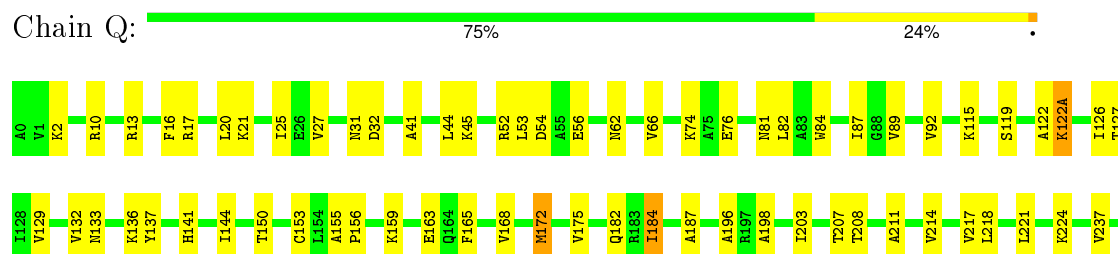
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

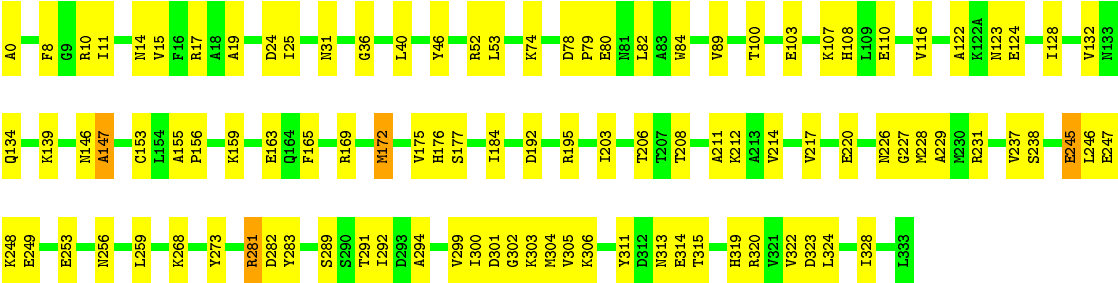


• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





● Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.87Å 124.80Å 82.92Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	8.00 – 2.45	Depositor
% Data completeness (in resolution range)	93.0 (8.00-2.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10559	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	O	0.56	0/2548	0.79	2/3454 (0.1%)
1	P	0.53	0/2548	0.78	3/3454 (0.1%)
1	Q	0.58	0/2548	0.79	2/3454 (0.1%)
1	R	0.57	0/2548	0.80	2/3454 (0.1%)
All	All	0.56	0/10192	0.79	9/13816 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	203	ILE	N-CA-C	-6.22	94.20	111.00
1	P	175	VAL	N-CA-C	-6.16	94.38	111.00
1	Q	175	VAL	N-CA-C	-6.12	94.49	111.00
1	P	203	ILE	N-CA-C	-5.98	94.86	111.00
1	O	175	VAL	N-CA-C	-5.85	95.19	111.00
1	Q	203	ILE	N-CA-C	-5.27	96.77	111.00
1	P	233	PRO	N-CA-C	5.25	125.76	112.10
1	O	203	ILE	N-CA-C	-5.14	97.13	111.00
1	R	175	VAL	N-CA-C	-5.02	97.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2513	0	2555	75	0
1	P	2513	0	2555	63	0
1	Q	2513	0	2555	58	0
1	R	2513	0	2555	70	0
2	O	10	0	0	0	0
2	P	10	0	0	0	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	O	44	0	26	3	0
3	P	44	0	26	1	0
3	Q	44	0	26	4	0
3	R	44	0	26	1	0
4	O	81	0	0	2	0
4	P	77	0	0	2	0
4	Q	66	0	0	2	0
4	R	67	0	0	0	0
All	All	10559	0	10324	248	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 12.

All (248) 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:O:2:LYS:HE2	1:O:28:VAL:HG11	1.53	0.90
1:Q:300:ILE:HG22	1:Q:304:MET:HB3	1.54	0.90
1:Q:159:LYS:HB3	1:Q:218:LEU:HD11	1.61	0.83
1:P:240:VAL:HG23	1:P:311:TYR:HE1	1.45	0.81
1:Q:187:ALA:O	1:Q:196:ALA:HB1	1.83	0.78
1:Q:306:LYS:HE2	1:R:228:MET:HG2	1.65	0.77
1:O:1:VAL:HB	1:O:25:ILE:HG22	1.66	0.75
1:P:240:VAL:HG23	1:P:311:TYR:CE1	2.23	0.73
1:O:104:ASP:O	1:O:107:LYS:HG2	1.89	0.72
1:P:139:LYS:HA	1:P:139:LYS:HE2	1.70	0.72
1:O:90:ASP:HB3	1:O:333:LEU:HD21	1.72	0.70
1:Q:165:PHE:HA	1:Q:248:LYS:HD3	1.74	0.70
1:O:184:ILE:H	1:O:184:ILE:HD12	1.56	0.69
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.28	0.69
1:R:212:LYS:H	1:R:212:LYS:HD2	1.56	0.69
1:O:182:GLN:HB3	4:O:355:HOH:O	1.92	0.68
1:Q:159:LYS:O	1:Q:163:GLU:HG3	1.92	0.68
1:O:157:PHE:HE1	1:O:242:LEU:HD23	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:87:ILE:HG13	1:Q:89:VAL:HG23	1.75	0.67
1:Q:56:GLU:O	1:Q:66:VAL:HA	1.93	0.67
1:Q:221:LEU:HA	1:Q:224:LYS:HD2	1.77	0.66
1:O:279:VAL:HG11	1:P:204:ILE:HG12	1.78	0.66
1:R:315:THR:O	1:R:319:HIS:HD2	1.78	0.64
1:O:160:VAL:O	1:O:164:GLN:HB2	1.97	0.64
1:P:172:MET:HG2	1:P:173:THR:N	2.12	0.64
1:P:176:HIS:HB3	1:P:231:ARG:HD3	1.79	0.64
1:R:299:VAL:HG22	1:R:305:VAL:HG23	1.80	0.63
1:P:166:GLY:O	1:P:246:LEU:HA	1.97	0.63
1:O:251:THR:O	1:O:255:VAL:HG23	1.99	0.62
1:R:176:HIS:O	1:R:231:ARG:HA	2.00	0.62
1:R:155:ALA:HB3	1:R:156:PRO:HD3	1.83	0.61
1:O:78:ASP:HB3	1:O:80:GLU:OE2	1.99	0.61
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.35	0.61
1:R:172:MET:CE	1:R:208:THR:HG21	2.30	0.61
1:O:62:ASN:O	1:O:73:VAL:HB	2.00	0.60
1:Q:32:ASP:HA	3:Q:336:NAD:N3A	2.15	0.60
1:O:32:ASP:HA	3:O:336:NAD:N3A	2.16	0.60
1:O:45:LYS:HD3	1:O:57:VAL:HB	1.82	0.60
1:O:102:ARG:HB2	1:O:123:ASN:HB2	1.84	0.60
1:O:56:GLU:O	1:O:66:VAL:HA	2.03	0.59
1:P:251:THR:H	1:P:254:GLU:HB2	1.67	0.59
1:P:333:LEU:HD12	1:P:333:LEU:H	1.67	0.59
1:Q:168:VAL:CG2	1:Q:247:GLU:HG3	2.32	0.59
1:P:9:GLY:HA3	3:P:336:NAD:O5B	2.02	0.59
1:R:107:LYS:HA	1:R:110:GLU:HG3	1.84	0.59
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.85	0.59
1:Q:41:ALA:O	1:Q:45:LYS:HG2	2.03	0.59
1:O:67:ASN:HB2	4:O:391:HOH:O	2.03	0.58
1:P:184:ILE:HD11	1:Q:182:GLN:O	2.03	0.58
1:P:58:SER:OG	1:P:65:VAL:HB	2.03	0.58
1:O:281:ARG:HG2	1:O:281:ARG:HH11	1.69	0.57
1:R:36:GLY:O	1:R:40:LEU:HG	2.05	0.57
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.85	0.57
1:O:301:ASP:HB2	1:P:169:ARG:HD3	1.87	0.56
1:O:84:TRP:HB3	1:O:89:VAL:HB	1.87	0.56
1:O:240:VAL:HG23	1:O:311:TYR:CE1	2.39	0.56
1:Q:76:GLU:HG3	1:Q:81:ASN:O	2.05	0.56
1:P:78:ASP:HB3	4:P:386:HOH:O	2.05	0.56
1:Q:249:GLU:HG3	1:Q:303:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:126:ILE:HG12	1:Q:127:THR:N	2.20	0.56
1:P:249:GLU:HA	1:P:302:GLY:O	2.06	0.55
1:O:165:PHE:O	1:O:248:LYS:HG3	2.07	0.55
1:O:32:ASP:OD2	3:O:336:NAD:H1B	2.07	0.55
1:O:260:LYS:O	1:O:264:GLU:HG3	2.07	0.54
1:R:172:MET:HG3	1:R:227:GLY:HA3	1.89	0.54
1:O:271:LEU:HD12	1:O:290:SER:O	2.08	0.54
1:R:248:LYS:HD3	1:R:249:GLU:H	1.71	0.54
1:Q:159:LYS:HB3	1:Q:218:LEU:CD1	2.35	0.54
1:P:271:LEU:HD11	1:P:292:ILE:HD11	1.90	0.53
1:R:214:VAL:O	1:R:217:VAL:HG22	2.08	0.53
1:Q:129:VAL:HG23	1:Q:217:VAL:HG11	1.91	0.53
1:O:119:SER:O	1:O:120:ALA:HB2	2.08	0.53
1:O:249:GLU:HA	1:O:302:GLY:O	2.08	0.53
1:P:182:GLN:O	1:Q:184:ILE:HD11	2.09	0.53
1:O:256:ASN:HD21	1:O:297:THR:CB	2.22	0.52
1:R:79:PRO:HB2	1:R:107:LYS:HB3	1.91	0.52
1:R:289:SER:OG	1:R:320:ARG:HD2	2.09	0.52
1:P:107:LYS:HA	1:P:110:GLU:OE1	2.10	0.51
1:Q:31:ASN:ND2	1:Q:82:LEU:HD21	2.24	0.51
1:R:212:LYS:HD2	1:R:212:LYS:N	2.24	0.51
1:R:19:ALA:CB	1:R:25:ILE:HD11	2.40	0.51
1:O:79:PRO:HB2	1:O:107:LYS:CB	2.40	0.51
1:R:249:GLU:HA	1:R:302:GLY:O	2.11	0.51
1:R:153:CYS:SG	1:R:311:TYR:CD1	3.03	0.51
1:R:46:TYR:HE1	1:R:52:ARG:HH11	1.58	0.51
1:O:45:LYS:O	1:O:52:ARG:HA	2.11	0.50
1:O:57:VAL:HG22	1:O:66:VAL:HG22	1.93	0.50
1:Q:44:LEU:HG	1:Q:53:LEU:HD22	1.92	0.50
1:Q:25:ILE:HD13	1:Q:322:VAL:HG13	1.93	0.50
1:Q:300:ILE:HG23	1:R:169:ARG:HD2	1.92	0.50
1:R:159:LYS:O	1:R:163:GLU:HG3	2.11	0.50
1:Q:300:ILE:CG2	1:R:169:ARG:HD2	2.42	0.50
1:O:276:GLU:OE1	1:O:277:PRO:HD2	2.12	0.50
1:P:52:ARG:NH2	1:R:282:ASP:O	2.45	0.50
1:O:79:PRO:HB2	1:O:107:LYS:HB2	1.93	0.50
1:R:153:CYS:HG	1:R:311:TYR:HD1	1.58	0.50
1:O:115:LYS:NZ	1:O:141:HIS:O	2.40	0.50
1:O:157:PHE:CE1	1:O:242:LEU:HD23	2.41	0.50
1:Q:115:LYS:NZ	1:Q:141:HIS:O	2.37	0.50
1:Q:74:LYS:HE2	1:Q:82:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:249:GLU:HG2	1:Q:303:LYS:HG3	1.94	0.50
1:O:182:GLN:HG2	1:O:195:ARG:HG2	1.94	0.49
1:O:208:THR:HG22	1:O:228:MET:HA	1.94	0.49
1:P:259:LEU:HD13	1:P:292:ILE:HG21	1.93	0.49
1:R:212:LYS:HE3	1:R:226:ASN:OD1	2.12	0.49
1:R:172:MET:HE2	1:R:208:THR:HG21	1.93	0.49
1:R:176:HIS:HB3	1:R:231:ARG:HD3	1.95	0.49
1:R:165:PHE:O	1:R:247:GLU:HB2	2.13	0.49
1:R:14:ASN:ND2	1:R:314:GLU:HB3	2.27	0.49
1:Q:267:LEU:HB3	1:Q:271:LEU:HB3	1.93	0.49
1:R:84:TRP:HB3	1:R:89:VAL:HB	1.94	0.49
1:Q:133:ASN:HB2	1:Q:136:LYS:HE2	1.95	0.49
1:P:283:TYR:CE2	1:P:310:TRP:CD1	3.01	0.48
1:O:282:ASP:O	1:Q:52:ARG:NH2	2.47	0.48
1:O:87:ILE:HG13	1:O:89:VAL:HG23	1.95	0.48
1:R:220:GLU:H	1:R:220:GLU:CD	2.16	0.48
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.48	0.48
1:R:315:THR:O	1:R:319:HIS:CD2	2.63	0.48
1:R:273:TYR:CE1	1:R:294:ALA:HB2	2.49	0.48
1:O:259:LEU:HD13	1:O:292:ILE:HG21	1.96	0.48
1:R:320:ARG:HA	1:R:323:ASP:HB2	1.96	0.47
1:R:256:ASN:HB3	1:R:273:TYR:OH	2.13	0.47
1:P:76:GLU:HB2	1:P:82:LEU:CD2	2.44	0.47
1:R:206:THR:HG23	1:R:229:ALA:HB3	1.96	0.47
1:P:297:THR:HA	1:P:306:LYS:O	2.14	0.47
1:R:253:GLU:CD	1:R:253:GLU:H	2.16	0.47
1:Q:16:PHE:CE2	1:Q:27:VAL:HG11	2.50	0.47
1:P:180:ASN:HA	1:Q:184:ILE:HD12	1.97	0.47
1:R:74:LYS:HE3	1:R:82:LEU:O	2.15	0.47
1:P:78:ASP:OD1	1:P:80:GLU:HG2	2.15	0.47
1:Q:207:THR:HG23	4:Q:372:HOH:O	2.14	0.47
1:O:181:ASP:OD2	1:O:195:ARG:HD3	2.15	0.46
1:O:279:VAL:CG1	1:P:204:ILE:HG12	2.43	0.46
1:Q:25:ILE:CD1	1:Q:322:VAL:HG13	2.45	0.46
1:R:0:ALA:HB3	1:R:24:ASP:O	2.15	0.46
1:O:1:VAL:HG23	1:O:24:ASP:O	2.16	0.46
1:Q:137:TYR:HE1	1:Q:144:ILE:HD11	1.80	0.46
1:O:270:ILE:O	1:O:288:VAL:HB	2.15	0.46
1:P:102:ARG:HG3	1:P:123:ASN:O	2.15	0.46
1:Q:211:ALA:O	1:Q:214:VAL:HB	2.15	0.46
1:O:10:ARG:HH11	1:O:13:ARG:HH21	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:48:SER:O	1:R:281:ARG:NH1	2.47	0.46
1:P:272:ALA:HB3	1:P:291:THR:HG23	1.97	0.46
1:R:139:LYS:NZ	1:R:139:LYS:HB3	2.30	0.46
1:O:246:LEU:HD23	1:O:250:VAL:HG21	1.98	0.46
1:P:249:GLU:HG2	1:P:303:LYS:HD3	1.96	0.46
1:R:19:ALA:HB2	1:R:25:ILE:HD11	1.98	0.46
1:P:253:GLU:CD	1:P:253:GLU:H	2.19	0.46
1:O:194:ARG:HD3	1:P:277:PRO:O	2.16	0.46
1:P:260:LYS:HE2	1:P:264:GLU:OE2	2.16	0.46
1:O:256:ASN:ND2	1:O:297:THR:HG21	2.31	0.46
1:O:38:ASN:N	1:O:38:ASN:HD22	2.14	0.46
1:R:146:ASN:O	1:R:147:ALA:HB3	2.16	0.45
1:Q:182:GLN:HB3	4:Q:357:HOH:O	2.16	0.45
1:O:101:LYS:HA	1:O:122(A):LYS:HB3	1.97	0.45
1:P:272:ALA:O	1:P:292:ILE:HG12	2.16	0.45
1:P:269:GLY:O	1:P:288:VAL:HG12	2.16	0.45
1:P:63:ASN:ND2	1:P:73:VAL:H	2.15	0.45
1:O:186:ASP:HB2	1:R:10:ARG:NH1	2.32	0.45
1:Q:119:SER:O	3:Q:336:NAD:H6N	2.17	0.45
1:Q:168:VAL:HG23	1:Q:247:GLU:HG3	1.99	0.45
1:R:128:ILE:HD12	1:R:134:GLN:HA	1.98	0.45
1:O:218:LEU:HD13	1:O:221:LEU:HD12	1.98	0.45
1:R:247:GLU:O	1:R:303:LYS:HE2	2.16	0.45
1:R:305:VAL:HG22	1:R:306:LYS:N	2.32	0.45
1:O:136:LYS:HE2	1:O:136:LYS:HA	1.99	0.45
1:Q:251:THR:OG1	1:Q:254:GLU:HG3	2.17	0.45
1:P:162:HIS:CG	1:P:221:LEU:HD21	2.52	0.45
1:R:299:VAL:HA	1:R:304:MET:O	2.17	0.44
1:P:84:TRP:HE1	1:P:108:HIS:CE1	2.35	0.44
1:Q:32:ASP:OD2	3:Q:336:NAD:H1B	2.17	0.44
1:Q:32:ASP:HA	3:Q:336:NAD:C2A	2.47	0.44
1:R:139:LYS:HZ2	1:R:139:LYS:HB3	1.82	0.44
1:P:300:ILE:O	1:P:301:ASP:HB2	2.16	0.44
1:Q:122:ALA:O	1:Q:122(A):LYS:HD3	2.17	0.44
1:O:221:LEU:HA	1:O:221:LEU:HD23	1.79	0.44
1:O:42:HIS:HA	1:O:45:LYS:NZ	2.32	0.44
1:P:221:LEU:HA	1:P:224:LYS:HD3	1.99	0.44
1:Q:17:ARG:HG2	1:Q:53:LEU:HD13	1.99	0.44
1:Q:327:TYR:O	1:Q:328:ILE:C	2.55	0.44
1:R:283:TYR:HE2	1:R:291:THR:HG21	1.82	0.44
1:O:2:LYS:HE2	1:O:28:VAL:CG1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:42:HIS:HA	1:O:45:LYS:HZ1	1.81	0.44
1:P:331:LYS:HD3	1:P:331:LYS:HA	1.71	0.44
1:P:84:TRP:NE1	1:P:108:HIS:ND1	2.61	0.44
1:R:15:VAL:HG13	1:R:322:VAL:HG23	2.00	0.44
1:R:172:MET:HG2	1:R:211:ALA:HB2	2.00	0.44
1:O:176:HIS:HB3	1:O:231:ARG:HD3	2.00	0.44
1:P:33:THR:HG23	1:P:77:ARG:HH21	1.83	0.43
1:R:17:ARG:HG2	1:R:53:LEU:HD13	1.99	0.43
1:Q:10:ARG:HH11	1:Q:13:ARG:HH21	1.67	0.43
1:Q:84:TRP:NE1	1:Q:92:VAL:HG21	2.33	0.43
1:P:190:HIS:HB3	1:P:192:ASP:O	2.18	0.43
1:P:138(A):PRO:HB3	4:P:377:HOH:O	2.17	0.43
1:P:106:ALA:O	1:P:109:LEU:N	2.52	0.43
1:O:169:ARG:HG3	1:O:169:ARG:HH11	1.83	0.43
1:Q:168:VAL:HG22	1:Q:247:GLU:HG3	2.01	0.43
1:P:45:LYS:O	1:P:52:ARG:HA	2.19	0.43
1:P:36:GLY:O	1:P:40:LEU:HG	2.18	0.43
1:R:31:ASN:ND2	3:R:336:NAD:H2A	2.33	0.43
1:P:102:ARG:NH1	1:P:125:ASP:OD1	2.52	0.43
1:P:206:THR:HG23	1:P:229:ALA:HB3	2.00	0.42
1:O:101:LYS:HE3	1:O:103:GLU:HG2	1.99	0.42
1:R:82:LEU:HD13	1:R:84:TRP:CZ2	2.54	0.42
1:O:3:VAL:N	1:O:26:GLU:O	2.52	0.42
1:R:324:LEU:O	1:R:328:ILE:HG13	2.19	0.42
1:R:192:ASP:HB3	1:R:195:ARG:HB2	2.01	0.42
1:R:305:VAL:HG22	1:R:306:LYS:H	1.84	0.42
1:O:10:ARG:HG2	3:O:336:NAD:O2A	2.19	0.42
1:O:122(A):LYS:O	1:O:123:ASN:HB2	2.18	0.42
1:O:169:ARG:HD3	1:P:301:ASP:HB2	2.01	0.42
1:P:64:LEU:O	1:P:70:GLU:HA	2.19	0.42
1:P:89:VAL:CG1	1:P:92:VAL:HG23	2.49	0.42
1:O:114:LYS:HD3	1:O:333:LEU:HG	2.01	0.42
1:R:108:HIS:HB2	1:R:116:VAL:CG2	2.50	0.42
1:P:76:GLU:HB2	1:P:82:LEU:HD23	2.02	0.42
1:Q:260:LYS:HG3	1:Q:273:TYR:CD1	2.55	0.42
1:R:11:ILE:O	1:R:15:VAL:HG23	2.20	0.42
1:R:122:ALA:HB3	1:R:124:GLU:HB3	2.01	0.41
1:O:280:SER:HB3	1:P:203:ILE:HB	2.01	0.41
1:Q:20:LEU:HA	1:Q:20:LEU:HD23	1.85	0.41
1:Q:150:THR:O	1:Q:153:CYS:HB3	2.19	0.41
1:O:299:VAL:HG11	1:O:302:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:238:SER:HB2	1:R:311:TYR:CZ	2.56	0.41
1:Q:17:ARG:O	1:Q:20:LEU:HB2	2.21	0.41
1:Q:256:ASN:HD22	1:Q:256:ASN:HA	1.64	0.41
1:R:299:VAL:HG12	1:R:300:ILE:N	2.36	0.41
1:R:107:LYS:O	1:R:110:GLU:HB2	2.20	0.41
1:R:79:PRO:HA	1:R:82:LEU:CD1	2.51	0.41
1:P:245:GLU:O	1:P:246:LEU:HD12	2.21	0.41
1:R:248:LYS:CD	1:R:249:GLU:H	2.33	0.41
1:O:310:TRP:HZ2	1:P:205:PRO:HG2	1.84	0.41
1:O:297:THR:HA	1:O:306:LYS:O	2.21	0.41
1:O:168:VAL:HG12	1:O:169:ARG:HG2	2.02	0.41
1:R:245:GLU:OE2	1:R:303:LYS:HD3	2.21	0.41
1:O:278:LEU:O	1:P:194:ARG:NH1	2.51	0.41
1:Q:172:MET:CE	1:Q:208:THR:HG21	2.50	0.41
1:R:259:LEU:HD13	1:R:292:ILE:HG21	2.03	0.41
1:Q:132:VAL:HG22	1:Q:159:LYS:HD3	2.02	0.40
1:Q:16:PHE:CD2	1:Q:27:VAL:HG11	2.56	0.40
1:P:156:PRO:O	1:P:160:VAL:HG23	2.21	0.40
1:P:272:ALA:CB	1:P:291:THR:HG23	2.52	0.40
1:R:132:VAL:HG22	1:R:159:LYS:HD2	2.02	0.40
1:P:159:LYS:HB2	1:P:218:LEU:HD11	2.03	0.40
1:O:31:ASN:ND2	1:O:82:LEU:HD21	2.37	0.40
1:O:256:ASN:HB3	1:O:273:TYR:OH	2.20	0.40
1:R:289:SER:HG	1:R:320:ARG:HD2	1.85	0.40
1:P:56:GLU:O	1:P:66:VAL:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	O	332/334 (99%)	306 (92%)	24 (7%)	2 (1%)	30 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	332/334 (99%)	312 (94%)	17 (5%)	3 (1%)	21	25
1	Q	332/334 (99%)	303 (91%)	25 (8%)	4 (1%)	16	17
1	R	332/334 (99%)	308 (93%)	22 (7%)	2 (1%)	30	35
All	All	1328/1336 (99%)	1229 (92%)	88 (7%)	11 (1%)	24	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	237	VAL
1	R	237	VAL
1	O	186	ASP
1	O	237	VAL
1	P	198	ALA
1	P	237	VAL
1	P	133	ASN
1	Q	21	LYS
1	R	147	ALA
1	Q	198	ALA
1	Q	332	GLY

5.3.2 Protein sidechains ⓘ

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	O	269/269 (100%)	255 (95%)	14 (5%)	29	40
1	P	269/269 (100%)	258 (96%)	11 (4%)	37	52
1	Q	269/269 (100%)	261 (97%)	8 (3%)	48	65
1	R	269/269 (100%)	254 (94%)	15 (6%)	26	36
All	All	1076/1076 (100%)	1028 (96%)	48 (4%)	34	47

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	78	ASP
1	O	80	GLU
1	O	172	MET
1	O	174	THR
1	O	184	ILE
1	O	218	LEU
1	O	220	GLU
1	O	246	LEU
1	O	253	GLU
1	O	280	SER
1	O	281	ARG
1	O	290	SER
1	O	305	VAL
1	O	331	LYS
1	P	8	PHE
1	P	52	ARG
1	P	60	ASN
1	P	62	ASN
1	P	100	THR
1	P	102	ARG
1	P	103	GLU
1	P	159	LYS
1	P	172	MET
1	P	184	ILE
1	P	298	MET
1	Q	2	LYS
1	Q	54	ASP
1	Q	62	ASN
1	Q	122(A)	LYS
1	Q	172	MET
1	Q	184	ILE
1	Q	256	ASN
1	Q	333	LEU
1	R	8	PHE
1	R	78	ASP
1	R	80	GLU
1	R	100	THR
1	R	103	GLU
1	R	123	ASN
1	R	172	MET
1	R	177	SER
1	R	184	ILE
1	R	245	GLU

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Mol	Chain	Res	Type
1	R	246	LEU
1	R	268	LYS
1	R	281	ARG
1	R	301	ASP
1	R	313	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	38	ASN
1	O	146	ASN
1	O	152	ASN
1	O	256	ASN
1	P	63	ASN
1	P	146	ASN
1	P	152	ASN
1	P	180	ASN
1	P	256	ASN
1	P	319	HIS
1	Q	62	ASN
1	Q	63	ASN
1	Q	146	ASN
1	Q	152	ASN
1	Q	256	ASN
1	R	14	ASN
1	R	63	ASN
1	R	146	ASN
1	R	152	ASN
1	R	319	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	O	336	-	38,48,48	1.08	3 (7%)	47,73,73	2.12	17 (36%)
2	SO4	O	338	-	4,4,4	1.34	1 (25%)	6,6,6	1.25	1 (16%)
2	SO4	O	339	-	4,4,4	1.26	0	6,6,6	0.42	0
3	NAD	P	336	-	38,48,48	1.39	4 (10%)	47,73,73	2.26	13 (27%)
2	SO4	P	338	-	4,4,4	1.11	0	6,6,6	0.51	0
2	SO4	P	339	-	4,4,4	1.12	0	6,6,6	0.55	0
3	NAD	Q	336	-	38,48,48	1.05	2 (5%)	47,73,73	2.35	10 (21%)
2	SO4	Q	338	-	4,4,4	1.24	0	6,6,6	0.26	0
2	SO4	Q	339	-	4,4,4	1.64	1 (25%)	6,6,6	0.46	0
3	NAD	R	336	-	38,48,48	1.43	3 (7%)	47,73,73	2.63	14 (29%)
2	SO4	R	338	-	4,4,4	0.89	0	6,6,6	0.27	0
2	SO4	R	339	-	4,4,4	1.15	0	6,6,6	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	O	336	-	-	0/22/62/62	0/5/5/5
2	SO4	O	338	-	-	0/0/0/0	0/0/0/0
2	SO4	O	339	-	-	0/0/0/0	0/0/0/0
3	NAD	P	336	-	-	0/22/62/62	0/5/5/5
2	SO4	P	338	-	-	0/0/0/0	0/0/0/0
2	SO4	P	339	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	Q	336	-	-	0/22/62/62	0/5/5/5
2	SO4	Q	338	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	339	-	-	0/0/0/0	0/0/0/0
3	NAD	R	336	-	-	0/22/62/62	0/5/5/5
2	SO4	R	338	-	-	0/0/0/0	0/0/0/0
2	SO4	R	339	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	336	NAD	C5A-N7A	-2.25	1.31	1.39
2	O	338	SO4	O3-S	-2.07	1.40	1.47
2	Q	339	SO4	O2-S	-2.06	1.40	1.47
3	Q	336	NAD	C3N-C7N	2.12	1.53	1.50
3	P	336	NAD	O2B-C2B	2.22	1.48	1.43
3	O	336	NAD	O4D-C1D	2.23	1.44	1.41
3	P	336	NAD	O4B-C1B	2.51	1.44	1.41
3	Q	336	NAD	O4D-C1D	2.64	1.44	1.41
3	P	336	NAD	C2N-C3N	2.66	1.43	1.39
3	R	336	NAD	O4B-C1B	3.09	1.45	1.41
3	O	336	NAD	C3N-C7N	3.16	1.55	1.50
3	R	336	NAD	O4D-C1D	3.78	1.46	1.41
3	P	336	NAD	C3N-C7N	4.48	1.57	1.50
3	R	336	NAD	C3N-C7N	5.44	1.59	1.50

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	336	NAD	N3A-C2A-N1A	-10.95	120.51	128.89
3	R	336	NAD	N3A-C2A-N1A	-10.37	120.95	128.89
3	P	336	NAD	N3A-C2A-N1A	-8.97	122.03	128.89
3	O	336	NAD	N3A-C2A-N1A	-8.03	122.74	128.89
3	P	336	NAD	O7N-C7N-N7N	-5.85	114.37	122.59
3	Q	336	NAD	C4B-O4B-C1B	-5.05	104.17	109.72
3	R	336	NAD	O7N-C7N-N7N	-4.90	115.69	122.59
3	Q	336	NAD	O4B-C4B-C5B	-3.92	95.32	109.32
3	P	336	NAD	C2N-C3N-C4N	-3.64	114.24	118.29
3	P	336	NAD	C4B-O4B-C1B	-3.62	105.75	109.72
3	R	336	NAD	C2N-C3N-C4N	-3.53	114.36	118.29
3	R	336	NAD	C4B-O4B-C1B	-3.08	106.33	109.72
3	O	336	NAD	O3D-C3D-C4D	-3.02	102.00	111.05
3	R	336	NAD	C5B-C4B-C3B	-2.98	103.37	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	336	NAD	C4D-O4D-C1D	-2.93	106.50	109.72
3	O	336	NAD	O4B-C1B-N9A	-2.76	102.32	108.10
2	O	338	SO4	O4-S-O3	-2.65	98.19	108.98
3	O	336	NAD	O3D-C3D-C2D	-2.63	103.29	111.83
3	O	336	NAD	O7N-C7N-N7N	-2.53	119.03	122.59
3	O	336	NAD	O5D-PN-O1N	-2.44	100.14	109.62
3	Q	336	NAD	O5B-C5B-C4B	-2.41	100.24	109.12
3	O	336	NAD	C5N-C6N-N1N	-2.38	116.36	120.47
3	O	336	NAD	C4B-O4B-C1B	-2.15	107.35	109.72
3	P	336	NAD	C5N-C6N-N1N	-2.13	116.79	120.47
3	P	336	NAD	C5B-C4B-C3B	-2.12	106.78	115.21
3	P	336	NAD	C2N-C3N-C7N	2.16	125.59	119.31
3	O	336	NAD	C6N-C5N-C4N	2.19	122.75	119.44
3	P	336	NAD	C6N-C5N-C4N	2.20	122.76	119.44
3	O	336	NAD	C2N-C3N-C7N	2.23	125.79	119.31
3	Q	336	NAD	O3-PN-O5D	2.27	108.96	102.94
3	Q	336	NAD	O4D-C1D-N1N	2.32	110.68	108.13
3	O	336	NAD	N6A-C6A-N1A	2.36	124.26	119.20
3	R	336	NAD	C3N-C2N-N1N	2.42	123.15	120.36
3	R	336	NAD	C4A-C5A-N7A	2.49	111.77	109.48
3	R	336	NAD	O3-PA-O5B	2.55	109.71	102.94
3	P	336	NAD	C3N-C2N-N1N	2.63	123.39	120.36
3	P	336	NAD	O3-PA-O5B	2.63	109.92	102.94
3	O	336	NAD	O4D-C1D-N1N	2.71	111.11	108.13
3	Q	336	NAD	C2A-N1A-C6A	2.74	123.66	118.77
3	R	336	NAD	C5N-C4N-C3N	2.74	123.78	120.33
3	R	336	NAD	C2A-N1A-C6A	2.75	123.67	118.77
3	P	336	NAD	C3N-C7N-N7N	2.75	120.83	117.82
3	Q	336	NAD	O4B-C4B-C3B	2.77	110.73	105.15
3	O	336	NAD	C3N-C7N-N7N	2.79	120.87	117.82
3	P	336	NAD	O7N-C7N-C3N	2.83	122.67	119.59
3	Q	336	NAD	O3B-C3B-C4B	2.94	119.88	111.05
3	Q	336	NAD	C4A-C5A-N7A	3.24	112.46	109.48
3	R	336	NAD	C4D-O4D-C1D	3.25	113.30	109.72
3	O	336	NAD	PN-O3-PA	3.32	142.05	132.73
3	P	336	NAD	C4A-C5A-N7A	3.32	112.53	109.48
3	O	336	NAD	C4A-C5A-N7A	3.43	112.63	109.48
3	O	336	NAD	C2B-C1B-N9A	3.65	119.87	114.29
3	R	336	NAD	O4B-C1B-N9A	3.80	116.06	108.10
3	R	336	NAD	O4D-C1D-N1N	4.70	113.30	108.13
3	R	336	NAD	O7N-C7N-C3N	6.50	126.68	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	336	NAD	3	0
3	P	336	NAD	1	0
3	Q	336	NAD	4	0
3	R	336	NAD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.