Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:13 AM GMT

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PDB ID	:	3LC1
Title	:	Crystal Structure of H178N mutant of Glyceraldehyde-3-phosphate-dehydrogenase 1 (GAPDH 1) from Staphylococcus aureus MRSA252 complexed with NAD at 2.0 angstrom resolution.
Authors	:	Mukherjee, S.; Dutta, D.; Saha, B.; Das, A.K.
Deposited on	:	2010-01-09
Resolution	:	2.00 Å(reported)

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 2.00 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		2.9%
RSRZ outliers		6.0%

Worse　　　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
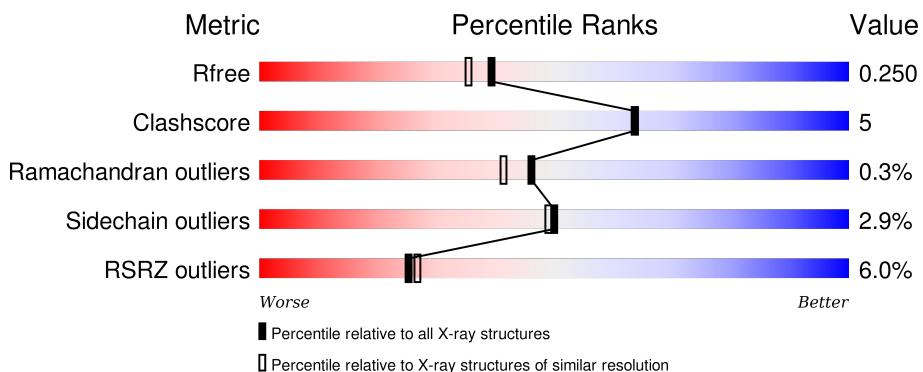
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	O	336	4% / 85% / 14% / ••
1	P	336	4% / 91% / 8% / •
1	Q	336	10% / 87% / 12% / ••
1	R	336	5% / 93% / 5% / •
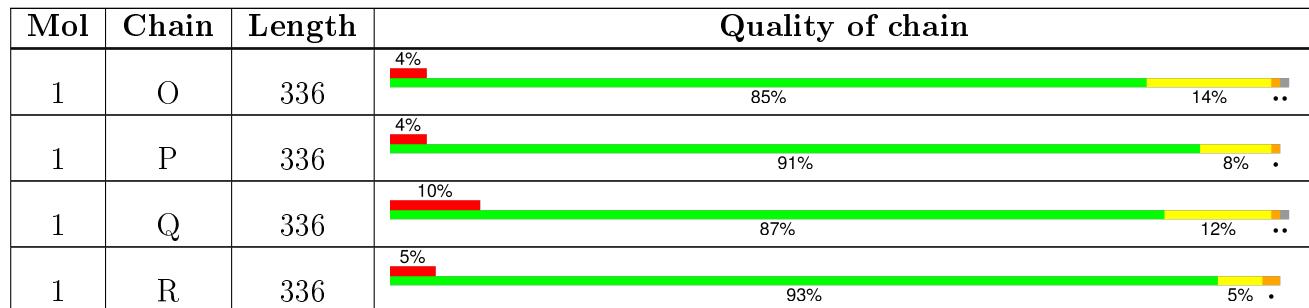
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	P	337	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10756 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	336	Total 2555	C 1590	N 440	O 515	S 10	0	2	0
1	R	336	Total 2552	C 1587	N 438	O 517	S 10	0	1	0
1	O	334	Total 2527	C 1572	N 434	O 512	S 9	0	0	0
1	Q	334	Total 2527	C 1572	N 434	O 512	S 9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	178	ASN	HIS	ENGINEERED	UNP Q6GIL8
R	178	ASN	HIS	ENGINEERED	UNP Q6GIL8
O	178	ASN	HIS	ENGINEERED	UNP Q6GIL8
Q	178	ASN	HIS	ENGINEERED	UNP Q6GIL8

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
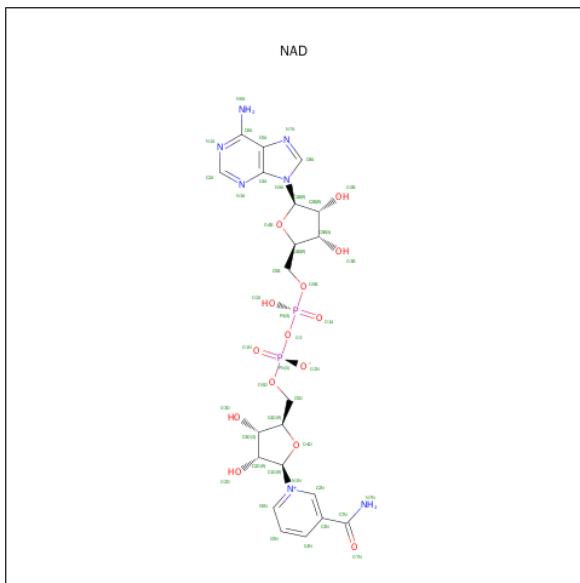
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
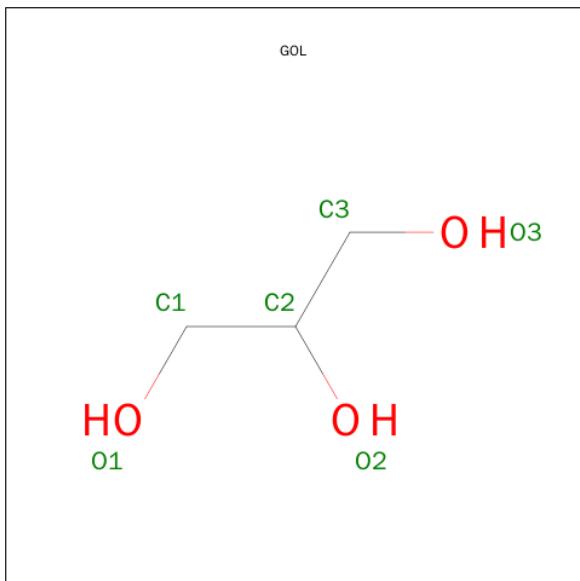
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	P	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	100	Total 100	O 100	0	0
4	R	111	Total 111	O 111	0	0
4	O	118	Total 118	O 118	0	0
4	Q	84	Total 84	O 84	0	0

3 Residue-property plots ⓘ

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.

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1
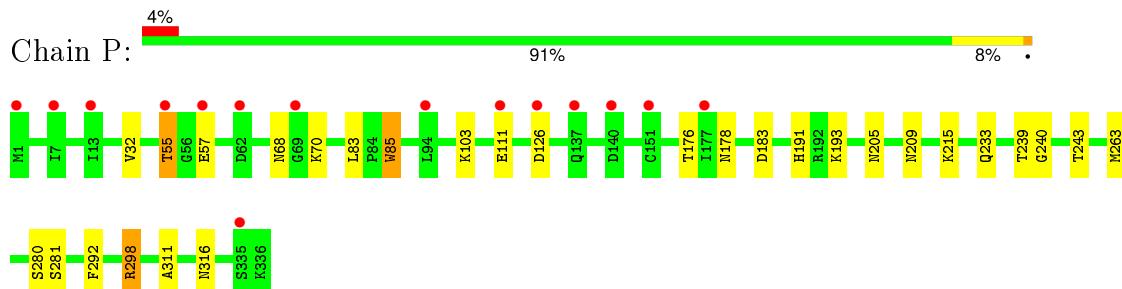
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1
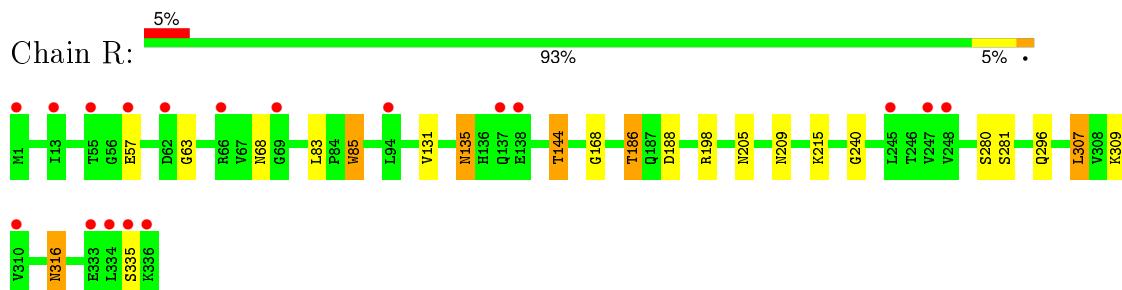
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1
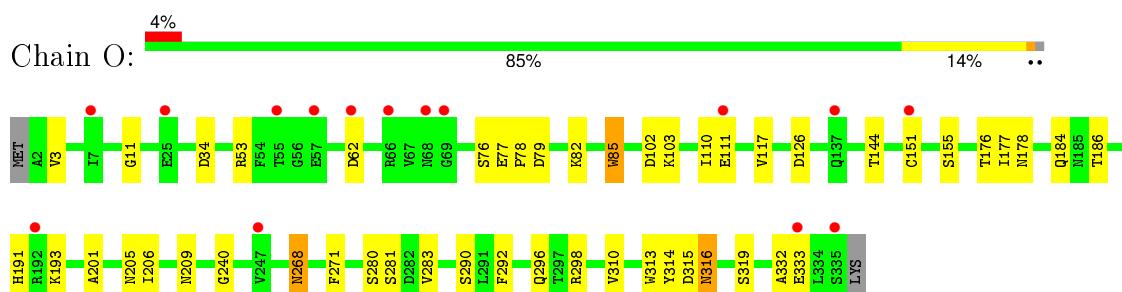
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1
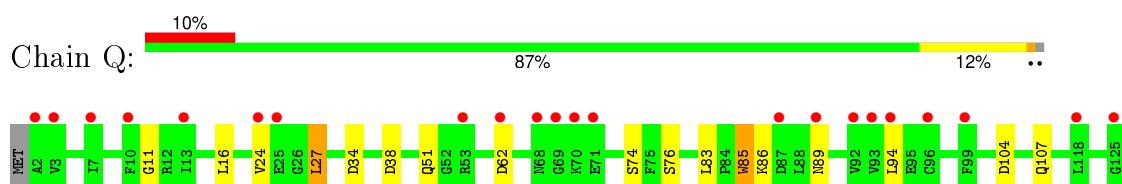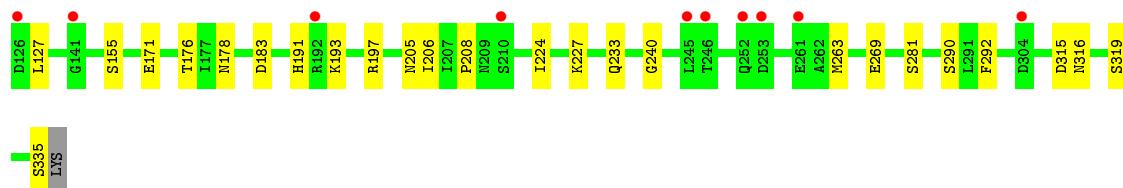
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.85Å 105.94Å 91.47Å 90.00° 108.34° 90.00°	Depositor
Resolution (Å)	29.06 – 2.00 29.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.06-2.00) 95.3 (29.06-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.56 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0095	Depositor
R, R_{free}	0.197 , 0.242 0.209 , 0.250	Depositor DCC
R_{free} test set	4003 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Outliers	0 of 80066 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10756	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 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	0.54	0/2560	0.64	0/3469
1	P	0.54	0/2594	0.63	0/3512
1	Q	0.52	0/2560	0.62	0/3469
1	R	0.56	0/2585	0.66	1/3501 (0.0%)
All	All	0.54	0/10299	0.64	1/13951 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	188	ASP	CB-CG-OD1	6.23	123.91	118.30

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	O	2527	0	2504	41	0
1	P	2555	0	2547	30	0
1	Q	2527	0	2504	26	0
1	R	2552	0	2532	25	0
2	O	44	0	26	1	0
2	P	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	44	0	26	1	0
2	R	44	0	26	0	0
3	P	6	0	8	0	0
4	O	118	0	0	5	0
4	P	100	0	0	2	0
4	Q	84	0	0	2	0
4	R	111	0	0	6	0
All	All	10756	0	10199	106	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 5.

All (106) 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:P:298[A]:ARG:HG3	1:P:298[A]:ARG:NH1	1.52	1.11
1:P:298[A]:ARG:CG	1:P:298[A]:ARG:HH11	1.64	1.07
1:R:144:THR:HG21	4:R:411:HOH:O	1.63	0.99
1:R:63:GLY:HA3	4:R:444:HOH:O	1.72	0.89
1:O:111:GLU:HG2	4:O:364:HOH:O	1.72	0.88
4:P:432:HOH:O	1:O:298:ARG:HD3	1.74	0.88
1:R:131:VAL:H	1:R:135:ASN:HD21	1.32	0.75
1:P:298[A]:ARG:HG3	1:P:298[A]:ARG:HH11	0.71	0.74
1:P:298[A]:ARG:CG	1:P:298[A]:ARG:NH1	2.35	0.71
1:P:183:ASP:O	1:P:191:HIS:HE1	1.75	0.69
1:Q:191:HIS:CD2	1:Q:193:LYS:H	2.13	0.66
1:R:131:VAL:H	1:R:135:ASN:ND2	1.96	0.64
1:Q:183:ASP:O	1:Q:191:HIS:HE1	1.81	0.64
1:Q:176:THR:HG23	1:Q:178:ASN:ND2	2.15	0.61
1:P:233:GLN:HG3	1:O:177:ILE:HD13	1.84	0.59
1:Q:38:ASP:OD1	1:Q:74:SER:OG	2.18	0.58
1:Q:224:ILE:HA	1:Q:227:LYS:HD2	1.84	0.58
1:R:198:ARG:NH1	4:R:390:HOH:O	2.38	0.57
1:Q:83:LEU:HD13	1:Q:85:TRP:CZ2	2.40	0.56
1:P:176:THR:HG23	1:P:178:ASN:ND2	2.20	0.56
1:P:191:HIS:CD2	1:P:193:LYS:H	2.24	0.55
1:P:57:GLU:H	1:P:68:ASN:ND2	2.03	0.55
1:R:186:THR:HG21	1:O:184:GLN:O	2.06	0.55
1:Q:240:GLY:H	1:Q:316:ASN:HD21	1.54	0.54
1:Q:24:VAL:HG11	1:Q:27:LEU:HD22	1.89	0.53
1:P:263:MET:HG3	1:P:292:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:268:ASN:ND2	1:O:271:PHE:H	2.06	0.53
1:R:186:THR:HG23	4:R:438:HOH:O	2.08	0.53
1:O:77:GLU:HG2	1:O:82:LYS:HB2	1.91	0.52
1:P:205:ASN:HD22	1:O:281:SER:H	1.58	0.51
1:P:240:GLY:H	1:P:316:ASN:HD21	1.58	0.51
1:O:103:LYS:HD2	1:O:126:ASP:O	2.11	0.51
1:Q:240:GLY:H	1:Q:316:ASN:ND2	2.09	0.50
1:P:83:LEU:HD13	1:P:85:TRP:CZ2	2.47	0.50
1:Q:104:ASP:O	1:Q:107:GLN:HB3	2.13	0.49
1:R:309:LYS:HE2	4:R:412:HOH:O	2.12	0.49
1:Q:269:GLU:HG2	4:Q:414:HOH:O	2.13	0.49
1:P:243:THR:O	1:P:311:ALA:HA	2.13	0.49
1:O:155:SER:HA	1:O:290:SER:HB2	1.94	0.49
1:Q:197:ARG:HD3	1:Q:208:PRO:O	2.13	0.48
1:O:240:GLY:H	1:O:316:ASN:ND2	2.11	0.48
1:P:263:MET:HG3	1:P:292:PHE:CE1	2.48	0.48
1:P:176:THR:HG23	1:P:178:ASN:HD21	1.79	0.48
1:O:268:ASN:C	1:O:268:ASN:HD22	2.17	0.48
1:O:176:THR:HG23	1:O:178:ASN:ND2	2.29	0.47
1:R:83:LEU:HD13	1:R:85:TRP:CZ2	2.50	0.47
1:P:281:SER:CB	1:O:205:ASN:HD21	2.28	0.47
1:R:281:SER:H	1:Q:205:ASN:HD22	1.63	0.47
1:O:3:VAL:HG21	1:O:332:ALA:HB1	1.97	0.47
1:O:240:GLY:H	1:O:316:ASN:HD21	1.63	0.46
1:O:292:PHE:HE1	1:O:310:VAL:HB	1.80	0.46
1:P:55:THR:HG22	4:P:371:HOH:O	2.15	0.46
1:Q:176:THR:CG2	1:Q:178:ASN:HD21	2.28	0.46
1:O:144:THR:HG21	4:O:393:HOH:O	2.15	0.46
1:O:144:THR:HG22	4:O:433:HOH:O	2.14	0.46
1:O:283:VAL:HG11	1:O:313:TRP:HB3	1.96	0.46
1:P:233:GLN:HG3	1:O:177:ILE:CD1	2.45	0.45
1:P:240:GLY:H	1:P:316:ASN:ND2	2.13	0.45
1:O:34:ASP:O	1:O:76:SER:HA	2.16	0.45
1:P:233:GLN:HE22	1:O:296:GLN:HE22	1.64	0.45
1:R:240:GLY:H	1:R:316:ASN:ND2	2.14	0.45
1:R:135:ASN:H	1:R:135:ASN:HD22	1.65	0.45
1:P:316:ASN:H	1:P:316:ASN:ND2	2.16	0.44
1:R:240:GLY:H	1:R:316:ASN:HD21	1.63	0.44
1:P:103:LYS:HD2	1:P:126:ASP:O	2.16	0.44
1:Q:176:THR:HG23	1:Q:178:ASN:HD21	1.82	0.44
1:P:233:GLN:HE22	1:O:296:GLN:NE2	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:215:LYS:HB3	1:R:215:LYS:HE2	1.66	0.44
1:O:268:ASN:HD22	1:O:271:PHE:H	1.65	0.44
1:O:280:SER:O	1:O:283:VAL:HG22	2.18	0.44
1:Q:263:MET:HG3	1:Q:292:PHE:CZ	2.53	0.44
1:R:280:SER:HB3	1:Q:206:ILE:HB	2.00	0.44
1:R:205:ASN:HD22	1:Q:281:SER:H	1.65	0.43
1:Q:155:SER:HA	1:Q:290:SER:HB2	2.00	0.43
1:R:135:ASN:HD22	1:R:135:ASN:N	2.17	0.43
1:O:316:ASN:H	1:O:316:ASN:ND2	2.17	0.43
1:R:85:TRP:HA	1:R:85:TRP:CE3	2.54	0.43
1:O:315:ASP:O	1:O:319:SER:HB2	2.18	0.43
1:R:57:GLU:H	1:R:68:ASN:ND2	2.16	0.43
1:R:316:ASN:ND2	1:R:316:ASN:H	2.17	0.43
1:O:191:HIS:CE1	1:O:193:LYS:HB2	2.54	0.43
1:R:85:TRP:HA	1:R:85:TRP:HE3	1.84	0.42
1:Q:191:HIS:HD2	1:Q:193:LYS:H	1.64	0.42
1:O:79:ASP:OD2	1:O:82:LYS:HE2	2.19	0.42
1:P:281:SER:H	1:O:205:ASN:ND2	2.17	0.42
1:R:68:ASN:HB2	4:R:370:HOH:O	2.19	0.42
1:O:110:ILE:HD11	1:O:117:VAL:HG23	2.02	0.42
1:Q:315:ASP:O	1:Q:319:SER:HB2	2.19	0.42
1:O:11:GLY:HA3	2:O:0:NAD:O5B	2.20	0.42
1:P:205:ASN:ND2	1:O:281:SER:H	2.18	0.41
1:Q:16:LEU:HD21	1:Q:51:GLN:HG3	2.01	0.41
1:O:53:ARG:HD3	4:Q:420:HOH:O	2.20	0.41
1:O:85:TRP:CE3	1:O:85:TRP:HA	2.55	0.41
1:O:193:LYS:HE2	4:O:389:HOH:O	2.20	0.41
1:Q:34:ASP:O	1:Q:76:SER:HA	2.20	0.41
1:P:281:SER:H	1:O:205:ASN:HD22	1.67	0.41
1:O:85:TRP:HE3	1:O:85:TRP:HA	1.84	0.41
1:R:131:VAL:N	1:R:135:ASN:HD21	2.10	0.41
1:P:85:TRP:HA	1:P:85:TRP:CE3	2.56	0.41
1:Q:11:GLY:HA3	2:Q:0:NAD:O5B	2.20	0.41
1:P:85:TRP:HA	1:P:85:TRP:HE3	1.85	0.41
1:P:280:SER:HB3	1:O:206:ILE:HB	2.02	0.41
1:O:151:CYS:SG	4:O:450:HOH:O	2.62	0.40
1:O:77:GLU:HA	1:O:78:PRO:HD2	1.98	0.40
1:R:307:LEU:HD22	1:Q:171:GLU:HG3	2.04	0.40
1:R:296:GLN:NE2	1:Q:233:GLN:HE22	2.20	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	O	332/336 (99%)	318 (96%)	13 (4%)	1 (0%)	46	41
1	P	336/336 (100%)	321 (96%)	15 (4%)	0	100	100
1	Q	332/336 (99%)	317 (96%)	14 (4%)	1 (0%)	46	41
1	R	335/336 (100%)	321 (96%)	12 (4%)	2 (1%)	30	22
All	All	1335/1344 (99%)	1277 (96%)	54 (4%)	4 (0%)	46	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	62	ASP
1	R	335	SER
1	O	201	ALA
1	R	168	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	O	272/274 (99%)	263 (97%)	9 (3%)	45	43
1	P	276/274 (101%)	266 (96%)	10 (4%)	42	39
1	Q	272/274 (99%)	265 (97%)	7 (3%)	54	54
1	R	275/274 (100%)	268 (98%)	7 (2%)	55	55
All	All	1095/1096 (100%)	1062 (97%)	33 (3%)	50	47

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	32	VAL
1	P	55	THR
1	P	70	LYS
1	P	85	TRP
1	P	111	GLU
1	P	209	ASN
1	P	215	LYS
1	P	239	THR
1	P	298[A]	ARG
1	P	298[B]	ARG
1	R	85	TRP
1	R	135	ASN
1	R	144	THR
1	R	186	THR
1	R	209	ASN
1	R	307	LEU
1	R	316	ASN
1	O	62	ASP
1	O	85	TRP
1	O	102	ASP
1	O	186	THR
1	O	209	ASN
1	O	268	ASN
1	O	314	TYR
1	O	316	ASN
1	O	333	GLU
1	Q	27	LEU
1	Q	85	TRP
1	Q	86	LYS
1	Q	89	ASN
1	Q	94	LEU
1	Q	127	LEU
1	Q	335	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	68	ASN
1	P	178	ASN
1	P	191	HIS
1	P	205	ASN

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Mol	Chain	Res	Type
1	P	252	GLN
1	P	316	ASN
1	R	68	ASN
1	R	135	ASN
1	R	178	ASN
1	R	205	ASN
1	R	265	ASN
1	R	296	GLN
1	R	316	ASN
1	O	178	ASN
1	O	205	ASN
1	O	265	ASN
1	O	268	ASN
1	O	296	GLN
1	O	316	ASN
1	Q	178	ASN
1	Q	191	HIS
1	Q	205	ASN
1	Q	265	ASN
1	Q	296	GLN
1	Q	316	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	#$\|Z\| > 2$
2	NAD	O	0	-	38,48,48	1.54	3 (7%)	47,73,73	2.15	6 (12%)
2	NAD	P	0	-	38,48,48	1.53	3 (7%)	47,73,73	2.24	7 (14%)
3	GOL	P	337	-	5,5,5	0.26	0	5,5,5	0.33	0
2	NAD	Q	0	-	38,48,48	1.54	3 (7%)	47,73,73	1.94	5 (10%)
2	NAD	R	0	-	38,48,48	1.55	3 (7%)	47,73,73	2.04	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	O	0	-	-	0/22/62/62	0/5/5/5
2	NAD	P	0	-	-	0/22/62/62	0/5/5/5
3	GOL	P	337	-	-	0/4/4/4	0/0/0/0
2	NAD	Q	0	-	-	0/22/62/62	0/5/5/5
2	NAD	R	0	-	-	0/22/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	0	NAD	C2A-N1A	2.23	1.38	1.33
2	P	0	NAD	C2A-N1A	2.36	1.38	1.33
2	O	0	NAD	C2A-N1A	2.47	1.38	1.33
2	R	0	NAD	C2A-N1A	2.50	1.38	1.33
2	R	0	NAD	C2A-N3A	3.17	1.37	1.32
2	O	0	NAD	C2A-N3A	3.48	1.38	1.32
2	Q	0	NAD	C2A-N3A	3.52	1.38	1.32
2	P	0	NAD	C2A-N3A	3.63	1.38	1.32
2	P	0	NAD	O7N-C7N	7.17	1.39	1.24
2	R	0	NAD	O7N-C7N	7.23	1.39	1.24
2	O	0	NAD	O7N-C7N	7.35	1.39	1.24
2	Q	0	NAD	O7N-C7N	7.45	1.40	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	0	NAD	N3A-C2A-N1A	-12.14	119.60	128.89
2	O	0	NAD	N3A-C2A-N1A	-11.56	120.04	128.89
2	R	0	NAD	N3A-C2A-N1A	-11.47	120.11	128.89
2	Q	0	NAD	N3A-C2A-N1A	-10.63	120.76	128.89
2	Q	0	NAD	PN-O3-PA	-3.19	123.78	132.73
2	O	0	NAD	PN-O3-PA	-2.87	124.67	132.73
2	O	0	NAD	O7N-C7N-C3N	-2.81	116.52	119.59
2	R	0	NAD	C1B-N9A-C4A	-2.70	122.87	126.94
2	P	0	NAD	C1B-N9A-C4A	-2.54	123.10	126.94
2	P	0	NAD	PN-O3-PA	-2.52	125.65	132.73
2	Q	0	NAD	O7N-C7N-C3N	-2.45	116.92	119.59
2	Q	0	NAD	C4A-C5A-N7A	-2.43	107.24	109.48
2	P	0	NAD	O7N-C7N-C3N	-2.39	116.98	119.59
2	P	0	NAD	C4A-C5A-N7A	-2.33	107.34	109.48
2	R	0	NAD	PN-O3-PA	-2.25	126.40	132.73
2	O	0	NAD	C1B-N9A-C4A	-2.20	123.62	126.94
2	R	0	NAD	O7N-C7N-N7N	-2.12	119.62	122.59
2	R	0	NAD	C3N-C7N-N7N	2.34	120.38	117.82
2	Q	0	NAD	C3N-C7N-N7N	2.80	120.88	117.82
2	R	0	NAD	O4D-C1D-N1N	3.48	111.95	108.13
2	O	0	NAD	C3N-C7N-N7N	4.02	122.22	117.82
2	P	0	NAD	O4D-C1D-N1N	4.04	112.57	108.13
2	O	0	NAD	O4D-C1D-N1N	4.07	112.61	108.13
2	P	0	NAD	C3N-C7N-N7N	4.31	122.53	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	0	NAD	1	0
2	Q	0	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 (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(Å²)	Q<0.9
1	O	334/336 (99%)	0.28	15 (4%)	37	38	20, 30, 45, 56	0
1	P	336/336 (100%)	0.35	15 (4%)	37	38	20, 31, 47, 64	0
1	Q	334/336 (99%)	0.59	32 (9%)	10	11	21, 34, 54, 63	0
1	R	336/336 (100%)	0.28	18 (5%)	29	31	21, 30, 44, 67	0
All	All	1340/1344 (99%)	0.38	80 (5%)	25	27	20, 31, 49, 67	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	335	SER	6.9
1	R	1	MET	6.0
1	R	336	LYS	4.9
1	Q	99	PHE	4.5
1	P	1	MET	4.2
1	O	62	ASP	3.8
1	Q	62	ASP	3.8
1	R	334	LEU	3.7
1	P	335	SER	3.7
1	Q	2	ALA	3.5
1	Q	304	ASP	3.5
1	Q	94	LEU	3.5
1	Q	126	ASP	3.5
1	O	55	THR	3.4
1	O	335	SER	3.4
1	R	66	ARG	3.4
1	Q	89	ASN	3.4
1	Q	25	GLU	3.3
1	P	126	ASP	3.3
1	P	94	LEU	3.2
1	Q	210	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	Q	69	GLY	3.0
1	R	62	ASP	2.9
1	P	55	THR	2.9
1	P	13	ILE	2.9
1	P	62	ASP	2.8
1	O	151	CYS	2.8
1	R	245	LEU	2.8
1	O	69	GLY	2.8
1	O	68	ASN	2.8
1	P	7	ILE	2.7
1	Q	253	ASP	2.7
1	Q	68	ASN	2.7
1	P	69	GLY	2.7
1	O	57	GLU	2.7
1	Q	125	GLY	2.6
1	R	55	THR	2.6
1	O	66	ARG	2.6
1	R	333	GLU	2.6
1	O	25	GLU	2.6
1	Q	261	GLU	2.6
1	Q	13	ILE	2.5
1	R	69	GLY	2.5
1	R	310	VAL	2.5
1	Q	7	ILE	2.5
1	P	57	GLU	2.5
1	O	247	VAL	2.5
1	Q	70	LYS	2.5
1	R	13	ILE	2.5
1	P	140	ASP	2.5
1	Q	3	VAL	2.5
1	Q	24	VAL	2.5
1	Q	92	VAL	2.4
1	P	137	GLN	2.4
1	P	111	GLU	2.4
1	Q	71	GLU	2.4
1	Q	96	CYS	2.4
1	R	57	GLU	2.4
1	Q	87	ASP	2.4
1	R	94	LEU	2.3
1	Q	53	ARG	2.3
1	P	177	ILE	2.3
1	O	7	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	192	ARG	2.3
1	Q	141	GLY	2.3
1	O	137	GLN	2.3
1	Q	246	THR	2.2
1	Q	93	VAL	2.2
1	Q	118	LEU	2.2
1	R	138	GLU	2.1
1	O	111	GLU	2.1
1	R	137	GLN	2.1
1	O	192	ARG	2.1
1	R	247	VAL	2.1
1	Q	10	PHE	2.0
1	R	248	VAL	2.0
1	Q	245	LEU	2.0
1	Q	252	GLN	2.0
1	P	151	CYS	2.0
1	O	333	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
3	GOL	P	337	6/6	0.53	0.34	11.15	54,55,56,57	0
2	NAD	O	0	44/44	0.93	0.13	-0.25	23,26,28,30	0
2	NAD	P	0	44/44	0.94	0.12	-0.44	21,28,33,35	0
2	NAD	R	0	44/44	0.96	0.11	-0.61	20,25,26,28	0
2	NAD	Q	0	44/44	0.95	0.10	-1.12	21,27,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.