



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K73  
Title : Crystal Structure of Phosphate bound Holo Glyceraldehyde-3-phosphate dehydrogenase 1 from MRSA252 at 2.5 Angstrom resolution  
Authors : Mukherjee, S.; Dutta, D.; Saha, B.; Das, A.K.  
Deposited on : 2009-10-12  
Resolution : 2.50 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

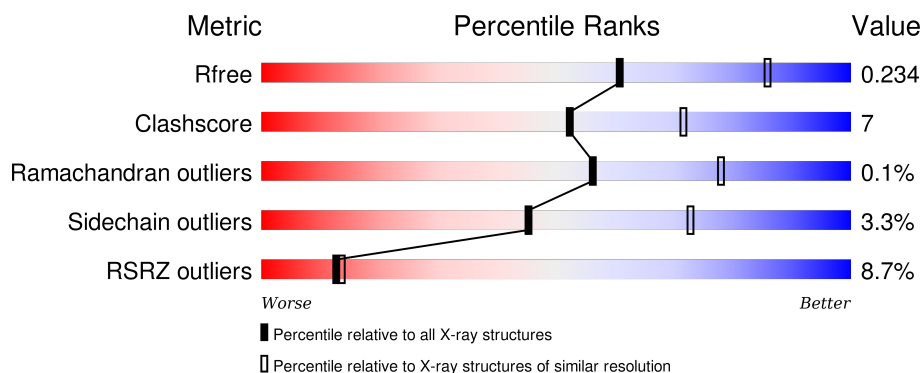
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	O	336	<div> <div>9%</div> <div>83%</div> <div>16%</div> </div>
1	P	336	<div> <div>6%</div> <div>85%</div> <div>14%</div> </div>
1	Q	336	<div> <div>8%</div> <div>85%</div> <div>15%</div> </div>
1	R	336	<div> <div>12%</div> <div>83%</div> <div>16%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10579 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	Q	336	Total	C	N	O	S	0	1	0
			2551	1588	438	515	10			
1	O	336	Total	C	N	O	S	0	0	0
			2546	1585	438	513	10			
1	P	336	Total	C	N	O	S	0	0	0
			2546	1585	438	513	10			
1	R	336	Total	C	N	O	S	0	0	0
			2546	1585	438	513	10			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



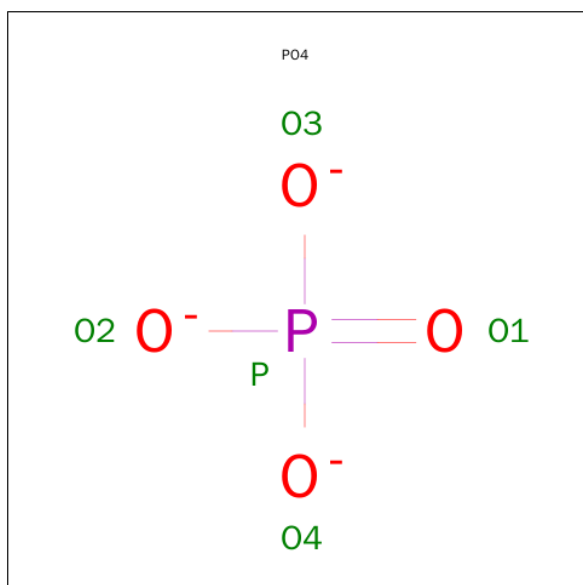
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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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		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

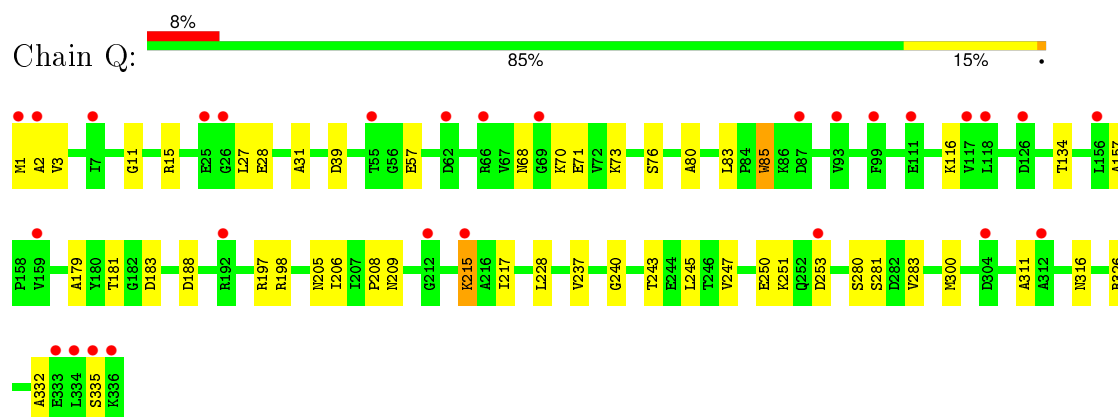
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	41	Total 41	O 41	0	0
4	O	45	Total 45	O 45	0	0
4	P	42	Total 42	O 42	0	0
4	R	46	Total 46	O 46	0	0

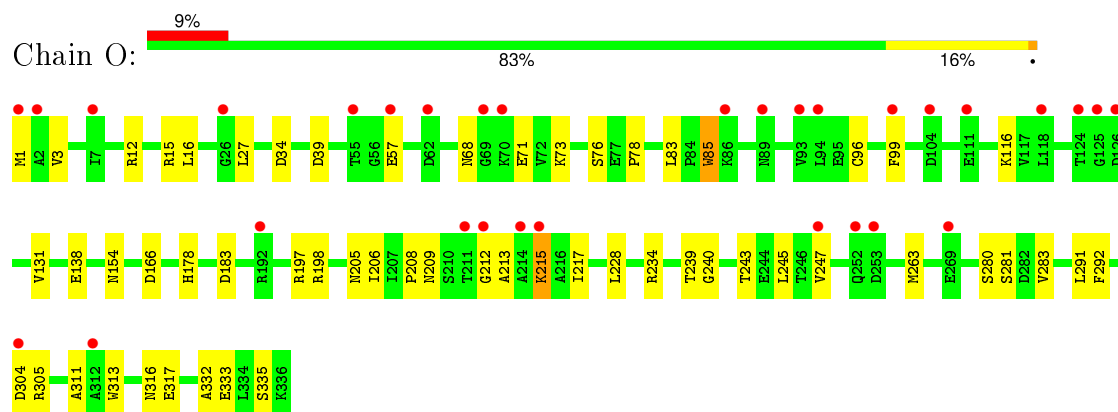
### 3 Residue-property plots

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.

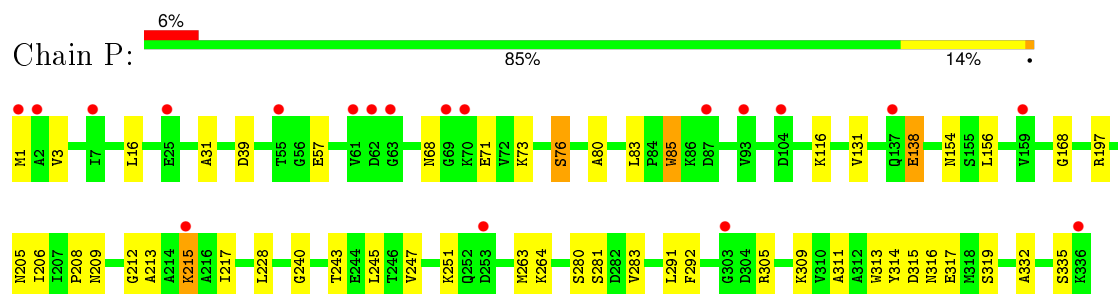
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



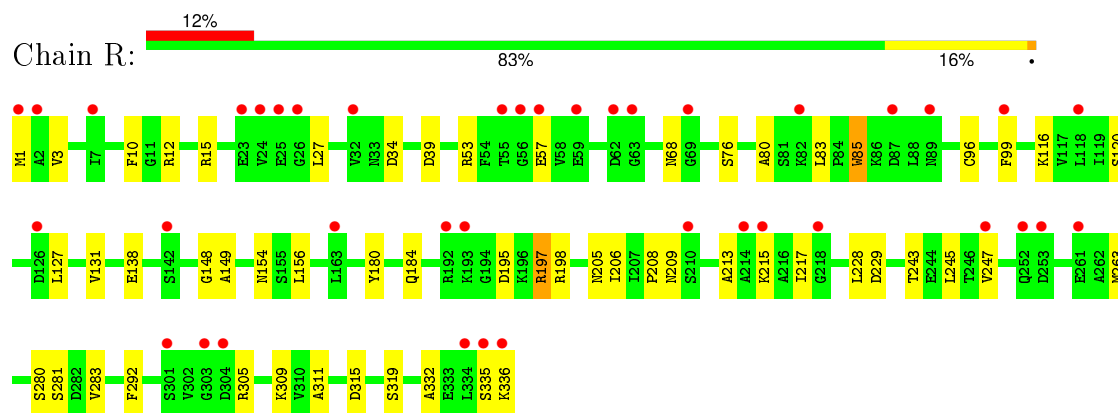
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.20 Å 104.85 Å 90.60 Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	19.14 – 2.50 19.14 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.14-2.50) 99.8 (19.14-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.49 Å)	Xtriage
Refinement program	REFMAC 5.5.0095	Depositor
R, $R_{free}$	0.177 , 0.224 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	2115 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 41927 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: PO4, 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	0.72	1/2580 (0.0%)	0.74	0/3494
1	P	0.72	0/2580	0.73	0/3494
1	Q	0.74	0/2588	0.75	2/3505 (0.1%)
1	R	0.70	0/2580	0.72	1/3494 (0.0%)
All	All	0.72	1/10328 (0.0%)	0.73	3/13987 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	96	CYS	CB-SG	-5.58	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	188	ASP	CB-CG-OD1	6.99	124.59	118.30
1	R	197	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	Q	326	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2546	0	2530	39	0
1	P	2546	0	2530	38	0
1	Q	2551	0	2534	36	0
1	R	2546	0	2530	39	0
2	O	44	0	26	4	0
2	P	44	0	26	1	0
2	Q	44	0	26	0	0
2	R	44	0	26	6	0
3	O	10	0	0	0	0
3	P	10	0	0	0	0
3	Q	10	0	0	0	0
3	R	10	0	0	0	0
4	O	45	0	0	5	0
4	P	42	0	0	8	0
4	Q	41	0	0	3	0
4	R	46	0	0	5	0
All	All	10579	0	10228	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (139) 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:304:ASP:HB2	4:O:340:HOH:O	1.46	1.13
1:R:198:ARG:HD3	4:R:339:HOH:O	1.62	1.00
1:O:198:ARG:HD3	4:O:339:HOH:O	1.64	0.95
1:Q:71:GLU:HB2	4:Q:372:HOH:O	1.71	0.90
1:O:34:ASP:HA	2:O:0:NAD:H8A	1.60	0.82
1:Q:253:ASP:HB3	4:Q:373:HOH:O	1.80	0.81
1:R:34:ASP:HA	2:R:0:NAD:H8A	1.67	0.77
1:Q:183[B]:ASP:OD2	1:Q:198:ARG:NH1	2.18	0.76
1:R:336:LYS:NZ	4:R:356:HOH:O	2.20	0.74
1:P:251:LYS:HG2	4:P:379:HOH:O	1.86	0.74
1:O:213:ALA:N	4:O:366:HOH:O	2.24	0.71
1:O:183:ASP:HB2	4:O:360:HOH:O	1.91	0.70
1:P:213:ALA:N	4:P:365:HOH:O	2.31	0.64
1:O:217:ILE:HG21	1:O:228:LEU:HD12	1.83	0.60
1:P:264:LYS:HD2	4:P:377:HOH:O	2.00	0.60
1:R:217:ILE:HG21	1:R:228:LEU:HD12	1.84	0.59
1:Q:28:GLU:OE1	1:Q:70:LYS:HE3	2.04	0.57
1:P:217:ILE:HG21	1:P:228:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:198:ARG:HD3	4:Q:339:HOH:O	2.05	0.57
1:Q:71:GLU:OE2	1:Q:73:LYS:HE3	2.05	0.57
1:Q:217:ILE:HG21	1:Q:228:LEU:HD12	1.86	0.56
1:Q:179:ALA:HB1	1:Q:237:VAL:O	2.05	0.56
1:P:316:ASN:O	2:P:0:NAD:H4N	2.06	0.55
1:R:34:ASP:OD2	2:R:0:NAD:H1B	2.07	0.55
1:P:309:LYS:CD	4:P:371:HOH:O	2.55	0.54
1:Q:181:THR:OG1	1:Q:183[A]:ASP:OD1	2.23	0.54
1:O:304:ASP:CB	4:O:340:HOH:O	2.26	0.54
1:Q:28:GLU:OE1	1:Q:70:LYS:NZ	2.41	0.53
1:P:243:THR:O	1:P:311:ALA:HA	2.10	0.52
1:O:263:MET:HG3	1:O:292:PHE:CZ	2.45	0.52
1:R:34:ASP:HA	2:R:0:NAD:C8A	2.37	0.52
1:P:3:VAL:HG21	1:P:332:ALA:HB1	1.90	0.52
1:O:78:PRO:HA	2:O:0:NAD:N6A	2.24	0.52
1:P:316:ASN:H	1:P:316:ASN:ND2	2.08	0.51
1:P:71:GLU:OE2	1:P:73:LYS:HE3	2.11	0.51
1:Q:205:ASN:HD22	1:R:281:SER:H	1.59	0.51
1:O:280:SER:O	1:O:283:VAL:HG22	2.10	0.51
1:P:156:LEU:HD23	1:P:217:ILE:HD13	1.92	0.51
1:R:3:VAL:HG21	1:R:332:ALA:HB1	1.93	0.51
1:Q:3:VAL:HB	1:Q:27:LEU:HD23	1.93	0.51
1:R:99:PHE:CD2	2:R:0:NAD:H2A	2.47	0.50
1:R:116:LYS:HE3	1:R:335:SER:HB2	1.93	0.50
1:P:76:SER:HB2	4:P:381:HOH:O	2.10	0.50
1:Q:31:ALA:HA	1:Q:73:LYS:O	2.12	0.49
1:Q:197:ARG:HD3	1:Q:208:PRO:O	2.11	0.49
1:O:240:GLY:H	1:O:316:ASN:HD21	1.59	0.49
1:R:3:VAL:HB	1:R:27:LEU:HD23	1.94	0.49
1:P:245:LEU:HG	1:P:247:VAL:HG13	1.95	0.49
1:P:197:ARG:HD3	1:P:208:PRO:O	2.12	0.49
1:O:263:MET:HG3	1:O:292:PHE:CE1	2.48	0.49
1:Q:11:GLY:O	1:Q:15:ARG:HG3	2.13	0.49
1:Q:28:GLU:OE1	1:Q:70:LYS:CE	2.60	0.48
1:Q:57:GLU:H	1:Q:68:ASN:ND2	2.10	0.48
1:O:243:THR:O	1:O:311:ALA:HA	2.14	0.48
1:O:57:GLU:H	1:O:68:ASN:ND2	2.12	0.48
1:R:243:THR:O	1:R:311:ALA:HA	2.14	0.48
1:P:57:GLU:H	1:P:68:ASN:ND2	2.12	0.48
1:O:71:GLU:OE2	1:O:73:LYS:HE3	2.14	0.48
1:Q:206:ILE:HB	1:R:280:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:215:LYS:HD2	1:O:215:LYS:HA	1.63	0.47
1:Q:116:LYS:HE3	1:Q:335:SER:HB2	1.96	0.47
1:O:240:GLY:H	1:O:316:ASN:ND2	2.12	0.47
1:P:315:ASP:O	1:P:319:SER:HB2	2.15	0.47
1:O:197:ARG:HD3	1:O:208:PRO:O	2.16	0.46
1:Q:215:LYS:HA	1:Q:215:LYS:HD2	1.52	0.46
1:R:180:TYR:HA	1:R:184:GLN:OE1	2.16	0.46
1:P:83:LEU:HD13	1:P:85:TRP:CZ2	2.51	0.46
1:P:212:GLY:O	1:P:213:ALA:C	2.52	0.46
1:R:99:PHE:CE2	2:R:0:NAD:H2A	2.50	0.46
1:Q:281:SER:H	1:R:205:ASN:HD22	1.64	0.46
1:O:3:VAL:HG21	1:O:332:ALA:HB1	1.98	0.46
1:Q:83:LEU:HD13	1:Q:85:TRP:CZ2	2.50	0.46
1:R:80:ALA:HA	1:R:83:LEU:HD12	1.98	0.46
1:Q:245:LEU:HG	1:Q:247:VAL:HG13	1.98	0.46
1:O:280:SER:HB3	1:P:206:ILE:HB	1.97	0.46
1:Q:80:ALA:HA	1:Q:83:LEU:HD12	1.98	0.46
1:Q:300:MET:CE	1:R:229:ASP:HB2	2.46	0.46
1:Q:243:THR:O	1:Q:311:ALA:HA	2.17	0.45
1:P:31:ALA:HA	1:P:73:LYS:O	2.16	0.45
1:P:116:LYS:HE3	1:P:335:SER:HB2	1.99	0.45
1:O:205:ASN:HD22	1:P:281:SER:H	1.64	0.45
1:R:53:ARG:NH1	4:R:362:HOH:O	2.50	0.45
1:P:215:LYS:HA	1:P:215:LYS:HD2	1.61	0.45
1:O:281:SER:H	1:P:205:ASN:HD22	1.65	0.45
1:Q:2:ALA:HB3	1:Q:28:GLU:HG2	1.99	0.45
1:O:16:LEU:CD1	1:O:317:GLU:HB3	2.47	0.45
1:Q:205:ASN:HD21	1:R:281:SER:CB	2.30	0.44
1:R:156:LEU:HD23	1:R:217:ILE:HD13	1.98	0.44
1:O:3:VAL:HB	1:O:27:LEU:HD23	1.99	0.44
1:O:83:LEU:HD13	1:O:85:TRP:CZ2	2.53	0.44
1:Q:3:VAL:HG21	1:Q:332:ALA:HB1	1.99	0.44
1:Q:251:LYS:HB2	1:Q:251:LYS:HE3	1.79	0.44
1:P:309:LYS:HD2	4:P:371:HOH:O	2.18	0.43
1:O:206:ILE:HB	1:P:280:SER:HB3	1.99	0.43
1:R:263:MET:HG3	1:R:292:PHE:CZ	2.53	0.43
1:R:96:CYS:HA	1:R:120:SER:OG	2.19	0.43
1:O:316:ASN:H	1:O:316:ASN:ND2	2.16	0.43
1:R:12:ARG:HH11	1:R:15:ARG:NH2	2.16	0.43
1:Q:280:SER:O	1:Q:283:VAL:HG22	2.19	0.43
1:P:80:ALA:HA	1:P:83:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:16:LEU:CD1	1:P:317:GLU:HB3	2.49	0.43
1:R:83:LEU:HD13	1:R:85:TRP:CZ2	2.54	0.43
1:O:281:SER:HB3	1:P:205:ASN:ND2	2.34	0.43
1:P:138:GLU:HG3	4:P:363:HOH:O	2.18	0.43
1:P:263:MET:HG3	1:P:292:PHE:CE1	2.54	0.43
1:O:34:ASP:HA	2:O:0:NAD:C8A	2.38	0.42
1:P:240:GLY:H	1:P:316:ASN:ND2	2.17	0.42
1:R:263:MET:HG3	1:R:292:PHE:CE1	2.54	0.42
1:Q:205:ASN:ND2	1:R:281:SER:H	2.16	0.42
1:R:245:LEU:HG	1:R:247:VAL:HG13	2.01	0.42
1:P:131:VAL:HG13	1:P:154:ASN:OD1	2.20	0.42
1:Q:240:GLY:H	1:Q:316:ASN:ND2	2.17	0.42
1:O:178:HIS:HB3	1:O:234:ARG:HD3	2.02	0.42
1:O:281:SER:CB	1:P:205:ASN:HD21	2.32	0.42
1:P:291:LEU:HB3	1:P:313:TRP:HB2	2.02	0.42
1:R:131:VAL:HG13	1:R:154:ASN:OD1	2.20	0.42
1:R:57:GLU:H	1:R:68:ASN:ND2	2.17	0.41
1:Q:280:SER:HB3	1:R:206:ILE:HB	2.01	0.41
1:O:116:LYS:HE3	1:O:335:SER:HB2	2.01	0.41
1:O:12:ARG:HH11	1:O:15:ARG:NH2	2.17	0.41
1:O:131:VAL:HG13	1:O:154:ASN:OD1	2.21	0.41
1:R:309:LYS:HD3	4:R:360:HOH:O	2.19	0.41
1:R:335:SER:HA	4:R:342:HOH:O	2.21	0.41
1:P:280:SER:O	1:P:283:VAL:HG22	2.21	0.41
1:O:99:PHE:CD2	2:O:0:NAD:H2A	2.56	0.41
1:P:309:LYS:HD3	4:P:371:HOH:O	2.18	0.41
1:Q:316:ASN:H	1:Q:316:ASN:ND2	2.18	0.41
1:R:280:SER:O	1:R:283:VAL:HG22	2.21	0.41
1:P:263:MET:HG3	1:P:292:PHE:CZ	2.56	0.41
1:O:245:LEU:HG	1:O:247:VAL:HG13	2.02	0.41
1:O:212:GLY:O	1:O:213:ALA:C	2.59	0.41
1:R:315:ASP:O	1:R:319:SER:HB2	2.21	0.41
1:O:291:LEU:HB3	1:O:313:TRP:HB2	2.03	0.40
1:Q:134:THR:HG21	1:Q:157:ALA:HB1	2.02	0.40
1:R:195:ASP:OD1	1:R:195:ASP:C	2.60	0.40
1:O:305:ARG:HB3	1:O:305:ARG:HE	1.73	0.40
1:R:99:PHE:CD2	2:R:0:NAD:C2A	3.04	0.40
1:R:148:GLY:O	1:R:149:ALA:HB3	2.22	0.40
1:R:197:ARG:HD3	1:R:208:PRO:O	2.22	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	334/336 (99%)	319 (96%)	15 (4%)	0	100	100
1	P	334/336 (99%)	321 (96%)	12 (4%)	1 (0%)	46	68
1	Q	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
1	R	334/336 (99%)	317 (95%)	16 (5%)	1 (0%)	46	68
All	All	1337/1344 (100%)	1278 (96%)	57 (4%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	213	ALA
1	P	168	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	274/274 (100%)	264 (96%)	10 (4%)	42	69
1	P	274/274 (100%)	265 (97%)	9 (3%)	45	73
1	Q	275/274 (100%)	268 (98%)	7 (2%)	55	82
1	R	274/274 (100%)	264 (96%)	10 (4%)	42	69
All	All	1097/1096 (100%)	1061 (97%)	36 (3%)	45	73

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	1	MET
1	Q	39	ASP
1	Q	76	SER
1	Q	85	TRP
1	Q	209	ASN
1	Q	215	LYS
1	Q	250	GLU
1	O	1	MET
1	O	39	ASP
1	O	76	SER
1	O	85	TRP
1	O	138	GLU
1	O	166	ASP
1	O	209	ASN
1	O	215	LYS
1	O	239	THR
1	O	333	GLU
1	P	1	MET
1	P	39	ASP
1	P	76	SER
1	P	85	TRP
1	P	138	GLU
1	P	209	ASN
1	P	215	LYS
1	P	305	ARG
1	P	314	TYR
1	R	1	MET
1	R	10	PHE
1	R	39	ASP
1	R	76	SER
1	R	85	TRP
1	R	127	LEU
1	R	138	GLU
1	R	209	ASN
1	R	215	LYS
1	R	305	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	43	HIS
1	Q	68	ASN
1	Q	205	ASN

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Mol	Chain	Res	Type
1	Q	316	ASN
1	O	68	ASN
1	O	205	ASN
1	O	316	ASN
1	P	68	ASN
1	P	205	ASN
1	P	316	ASN
1	R	68	ASN
1	R	205	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](#)

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$
2	NAD	O	0	-	38,48,48	1.99	4 (10%)	47,73,73	2.28	14 (29%)
3	PO4	O	337	-	4,4,4	0.39	0	6,6,6	0.27	0
3	PO4	O	338	-	4,4,4	0.37	0	6,6,6	0.28	0
2	NAD	P	0	-	38,48,48	1.71	5 (13%)	47,73,73	2.13	9 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	P	337	-	4,4,4	0.39	0	6,6,6	0.30	0
3	PO4	P	338	-	4,4,4	0.48	0	6,6,6	0.26	0
2	NAD	Q	0	-	38,48,48	1.67	4 (10%)	47,73,73	2.43	9 (19%)
3	PO4	Q	337	-	4,4,4	0.44	0	6,6,6	0.27	0
3	PO4	Q	338	-	4,4,4	0.20	0	6,6,6	0.28	0
2	NAD	R	0	-	38,48,48	1.78	4 (10%)	47,73,73	1.89	7 (14%)
3	PO4	R	337	-	4,4,4	0.31	0	6,6,6	0.29	0
3	PO4	R	338	-	4,4,4	0.25	0	6,6,6	0.31	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
2	NAD	O	0	-	-	0/22/62/62	0/5/5/5
3	PO4	O	337	-	-	0/0/0/0	0/0/0/0
3	PO4	O	338	-	-	0/0/0/0	0/0/0/0
2	NAD	P	0	-	-	0/22/62/62	0/5/5/5
3	PO4	P	337	-	-	0/0/0/0	0/0/0/0
3	PO4	P	338	-	-	0/0/0/0	0/0/0/0
2	NAD	Q	0	-	-	0/22/62/62	0/5/5/5
3	PO4	Q	337	-	-	0/0/0/0	0/0/0/0
3	PO4	Q	338	-	-	0/0/0/0	0/0/0/0
2	NAD	R	0	-	-	0/22/62/62	0/5/5/5
3	PO4	R	337	-	-	0/0/0/0	0/0/0/0
3	PO4	R	338	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	0	NAD	O4B-C4B	-2.11	1.40	1.45
2	Q	0	NAD	PN-O2N	-2.10	1.46	1.54
2	P	0	NAD	O4B-C4B	-2.02	1.40	1.45
2	O	0	NAD	O2D-C2D	-2.00	1.38	1.43
2	Q	0	NAD	C2A-N1A	2.09	1.37	1.33
2	P	0	NAD	C2N-C3N	2.40	1.42	1.39
2	P	0	NAD	C2A-N1A	2.82	1.39	1.33
2	Q	0	NAD	C2A-N3A	3.01	1.37	1.32
2	P	0	NAD	C2A-N3A	3.44	1.38	1.32
2	R	0	NAD	C2A-N3A	3.47	1.38	1.32
2	O	0	NAD	C2A-N1A	3.91	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	0	NAD	C2A-N1A	3.92	1.41	1.33
2	O	0	NAD	C2A-N3A	4.55	1.40	1.32
2	Q	0	NAD	O7N-C7N	7.69	1.40	1.24
2	R	0	NAD	O7N-C7N	7.89	1.41	1.24
2	P	0	NAD	O7N-C7N	7.92	1.41	1.24
2	O	0	NAD	O7N-C7N	9.01	1.43	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	0	NAD	N3A-C2A-N1A	-13.32	118.69	128.89
2	P	0	NAD	N3A-C2A-N1A	-10.07	121.19	128.89
2	O	0	NAD	N3A-C2A-N1A	-7.65	123.03	128.89
2	R	0	NAD	N3A-C2A-N1A	-6.75	123.72	128.89
2	R	0	NAD	C4B-O4B-C1B	-5.15	104.06	109.72
2	O	0	NAD	C3N-C7N-N7N	-4.21	113.21	117.82
2	P	0	NAD	O7N-C7N-C3N	-4.19	115.01	119.59
2	R	0	NAD	PN-O3-PA	-4.08	121.28	132.73
2	O	0	NAD	PN-O3-PA	-3.11	124.00	132.73
2	Q	0	NAD	PN-O3-PA	-2.70	125.14	132.73
2	Q	0	NAD	O7N-C7N-N7N	-2.54	119.02	122.59
2	O	0	NAD	O3B-C3B-C4B	-2.44	103.72	111.05
2	Q	0	NAD	O5B-C5B-C4B	-2.44	100.13	109.12
2	P	0	NAD	O3-PN-O5D	-2.33	96.76	102.94
2	O	0	NAD	C3N-C2N-N1N	-2.19	117.84	120.36
2	Q	0	NAD	C5B-C4B-C3B	-2.16	106.62	115.21
2	P	0	NAD	O5B-C5B-C4B	-2.11	101.34	109.12
2	O	0	NAD	C4B-O4B-C1B	-2.10	107.42	109.72
2	P	0	NAD	C4N-C3N-C7N	-2.09	115.56	121.09
2	O	0	NAD	C5N-C4N-C3N	-2.09	117.71	120.33
2	O	0	NAD	C4N-C3N-C7N	-2.07	115.61	121.09
2	P	0	NAD	C1B-N9A-C4A	-2.05	123.84	126.94
2	Q	0	NAD	O2N-PN-O3	2.15	114.84	105.09
2	P	0	NAD	O3-PA-O5B	2.25	108.90	102.94
2	O	0	NAD	O4B-C1B-N9A	2.50	113.33	108.10
2	R	0	NAD	C2N-C3N-C4N	2.51	121.08	118.29
2	P	0	NAD	O4D-C1D-N1N	2.65	111.05	108.13
2	Q	0	NAD	C3N-C7N-N7N	2.87	120.95	117.82
2	Q	0	NAD	O4D-C1D-N1N	2.92	111.33	108.13
2	O	0	NAD	O7N-C7N-N7N	2.95	126.74	122.59
2	R	0	NAD	O4B-C1B-N9A	3.01	114.40	108.10
2	R	0	NAD	O4D-C1D-N1N	3.05	111.48	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	0	NAD	O4D-C1D-N1N	3.13	111.57	108.13
2	Q	0	NAD	C4D-O4D-C1D	3.91	114.02	109.72
2	O	0	NAD	C1B-N9A-C4A	3.94	132.88	126.94
2	P	0	NAD	C3N-C7N-N7N	4.17	122.38	117.82
2	O	0	NAD	C2N-C3N-C4N	4.18	122.95	118.29
2	R	0	NAD	C2B-C1B-N9A	5.18	122.21	114.29
2	O	0	NAD	C2B-C1B-N9A	6.85	124.76	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	0	NAD	4	0
2	P	0	NAD	1	0
2	R	0	NAD	6	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	336/336 (100%)	0.48	31 (9%)	11 12	41, 59, 82, 100	0
1	P	336/336 (100%)	0.36	19 (5%)	27 31	40, 56, 79, 98	0
1	Q	336/336 (100%)	0.44	28 (8%)	14 15	41, 59, 81, 98	0
1	R	336/336 (100%)	0.62	39 (11%)	6 6	39, 63, 91, 113	0
All	All	1344/1344 (100%)	0.47	117 (8%)	13 13	39, 59, 84, 113	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	1	MET	9.0
1	O	1	MET	8.9
1	Q	1	MET	8.6
1	Q	336	LYS	8.0
1	R	1	MET	7.1
1	R	304	ASP	7.0
1	R	2	ALA	6.7
1	R	336	LYS	6.7
1	R	214	ALA	6.6
1	P	336	LYS	5.4
1	P	62	ASP	5.2
1	Q	304	ASP	5.0
1	P	55	THR	4.9
1	O	126	ASP	4.8
1	P	2	ALA	4.7
1	Q	2	ALA	4.4
1	O	2	ALA	4.3
1	R	62	ASP	4.2
1	Q	62	ASP	4.1
1	R	87	ASP	4.1
1	R	99	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	Q	25	GLU	4.0
1	R	252	GLN	3.9
1	O	62	ASP	3.9
1	Q	26	GLY	3.8
1	O	304	ASP	3.7
1	R	218	GLY	3.7
1	R	25	GLU	3.7
1	R	335	SER	3.6
1	R	247	VAL	3.6
1	O	94	LEU	3.5
1	O	26	GLY	3.5
1	R	82	LYS	3.5
1	Q	334	LEU	3.5
1	Q	335	SER	3.5
1	O	57	GLU	3.3
1	O	252	GLN	3.3
1	O	55	THR	3.3
1	P	87	ASP	3.3
1	Q	55	THR	3.3
1	Q	126	ASP	3.3
1	O	253	ASP	3.3
1	Q	93	VAL	3.2
1	Q	7	ILE	3.1
1	Q	333	GLU	3.1
1	O	124	THR	3.1
1	P	63	GLY	3.1
1	Q	192	ARG	3.1
1	R	7	ILE	3.1
1	P	159	VAL	3.0
1	P	93	VAL	3.0
1	O	125	GLY	2.9
1	R	192	ARG	2.9
1	O	99	PHE	2.9
1	R	55	THR	2.9
1	O	70	LYS	2.9
1	Q	117	VAL	2.8
1	O	215	LYS	2.8
1	R	59	GLU	2.8
1	Q	253	ASP	2.7
1	O	214	ALA	2.7
1	Q	111	GLU	2.7
1	Q	312	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	192	ARG	2.6
1	R	303	GLY	2.6
1	P	61	VAL	2.6
1	R	301	SER	2.6
1	Q	66	ARG	2.6
1	R	89	ASN	2.6
1	O	7	ILE	2.5
1	R	126	ASP	2.5
1	O	118	LEU	2.5
1	R	24	VAL	2.5
1	O	111	GLU	2.5
1	R	193	LYS	2.5
1	P	137	GLN	2.5
1	R	215	LYS	2.4
1	O	89	ASN	2.4
1	R	210	SER	2.4
1	R	63	GLY	2.4
1	R	163	LEU	2.4
1	O	211	THR	2.4
1	O	93	VAL	2.4
1	Q	212	GLY	2.3
1	O	69	GLY	2.3
1	Q	159	VAL	2.3
1	R	142	SER	2.3
1	Q	99	PHE	2.3
1	Q	118	LEU	2.3
1	O	247	VAL	2.3
1	O	312	ALA	2.3
1	Q	156	LEU	2.3
1	R	23	GLU	2.2
1	O	212	GLY	2.2
1	R	253	ASP	2.2
1	Q	69	GLY	2.2
1	O	86	LYS	2.2
1	Q	215	LYS	2.2
1	P	215	LYS	2.2
1	P	25	GLU	2.2
1	R	69	GLY	2.1
1	P	253	ASP	2.1
1	R	118	LEU	2.1
1	R	56	GLY	2.1
1	P	7	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	334	LEU	2.1
1	R	261	GLU	2.1
1	R	26	GLY	2.1
1	P	303	GLY	2.1
1	O	104	ASP	2.1
1	Q	87	ASP	2.0
1	P	104	ASP	2.0
1	R	57	GLU	2.0
1	P	70	LYS	2.0
1	P	69	GLY	2.0
1	R	32	VAL	2.0
1	O	269	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PO4	Q	338	5/5	0.95	0.19	1.73	75,76,79,81	0
3	PO4	R	337	5/5	0.93	0.19	0.63	79,82,89,89	0
3	PO4	P	338	5/5	0.91	0.19	0.56	91,94,98,100	0
3	PO4	O	338	5/5	0.95	0.20	0.55	80,83,87,88	0
2	NAD	O	0	44/44	0.95	0.15	-0.26	32,43,56,66	0
2	NAD	R	0	44/44	0.94	0.16	-0.30	32,45,51,57	0
3	PO4	Q	337	5/5	0.96	0.13	-0.64	83,87,89,92	0
2	NAD	Q	0	44/44	0.97	0.12	-0.87	37,43,49,50	0
2	NAD	P	0	44/44	0.97	0.12	-1.13	25,42,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	P	337	5/5	0.91	0.25	-	81,85,88,91	0
3	PO4	O	337	5/5	0.94	0.15	-	64,66,66,73	0
3	PO4	R	338	5/5	0.85	0.21	-	81,82,85,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.