



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:10 AM GMT

PDB ID : 3L4S  
Title : Crystal structure of C151G mutant of Glyceraldehyde 3-phosphate dehydrogenase 1 (GAPDH1) from methicillin resistant Staphylococcus aureus MRSA252 complexed with NAD and G3P  
Authors : Mukherjee, S.; Dutta, D.; Saha, B.; Das, A.K.  
Deposited on : 2009-12-21  
Resolution : 2.20 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

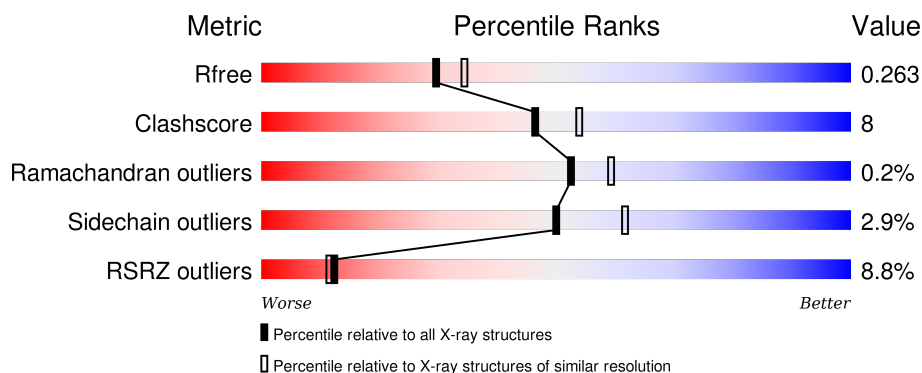
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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>84%</div> <div>14%</div> <div>..</div> </div>
1	P	336	<div> <div>10%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	Q	336	<div> <div>7%</div> <div>84%</div> <div>15%</div> <div>..</div> </div>
1	R	336	<div> <div>10%</div> <div>83%</div> <div>16%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10594 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.

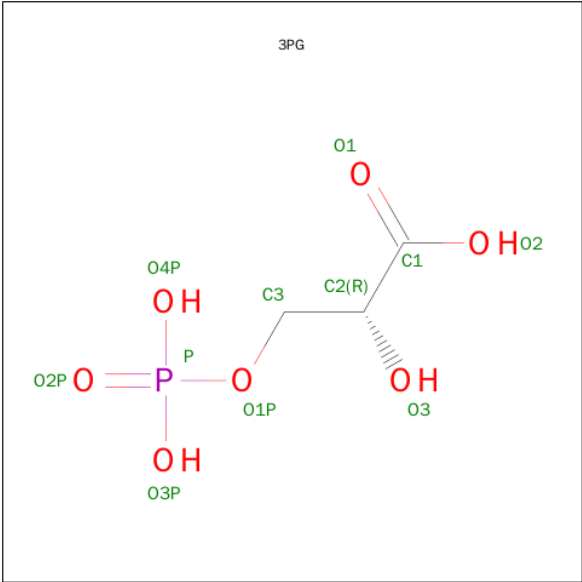
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	334	Total	C	N	O	S	0	0	0
			2529	1575	435	510	9			
1	P	333	Total	C	N	O	S	0	1	0
			2526	1573	434	511	8			
1	O	334	Total	C	N	O	S	0	0	0
			2529	1575	435	510	9			
1	R	334	Total	C	N	O	S	0	0	0
			2527	1573	435	511	8			

There are 4 discrepancies between the modelled and reference sequences:

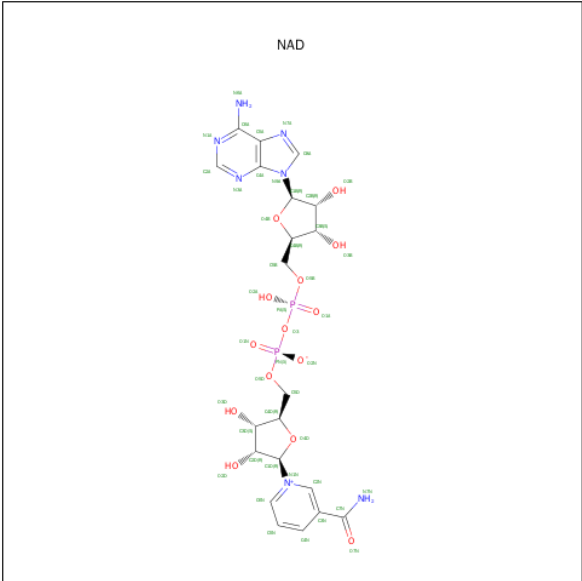
Chain	Residue	Modelled	Actual	Comment	Reference
Q	151	GLY	CYS	ENGINEERED	UNP Q6GIL8
P	151	GLY	CYS	ENGINEERED	UNP Q6GIL8
O	151	GLY	CYS	ENGINEERED	UNP Q6GIL8
R	151	GLY	CYS	ENGINEERED	UNP Q6GIL8

- Molecule 2 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Q	1	Total	C	O	P	0	0
			11	3	7	1		
2	P	1	Total	C	O	P	0	0
			11	3	7	1		
2	O	1	Total	C	O	P	0	0
			11	3	7	1		
2	R	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Q	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	O	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		

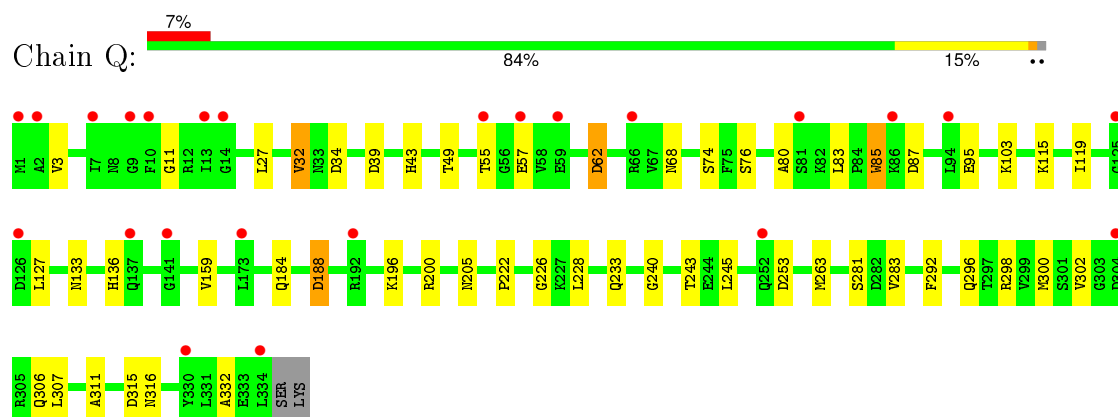
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	60	Total	O	0	0
			60	60		
4	P	62	Total	O	0	0
			62	62		
4	O	73	Total	O	0	0
			73	73		
4	R	68	Total	O	0	0
			68	68		

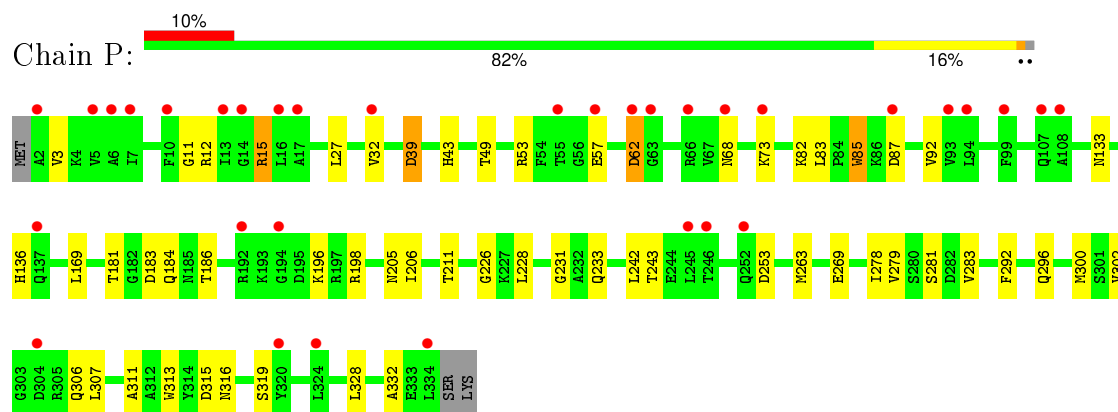
### 3 Residue-property plots [i](#)

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.

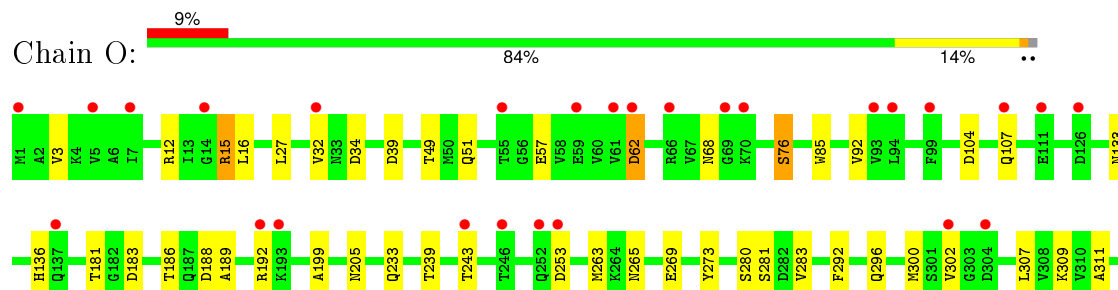
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1

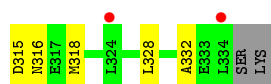


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1



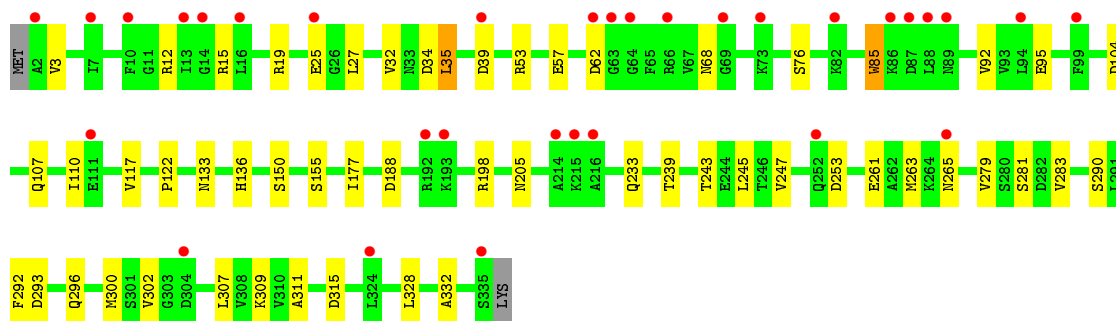
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1





- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase 1

Chain R: 10% 83% 16% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.59Å 102.94Å 90.65Å 90.00° 109.31° 90.00°	Depositor
Resolution (Å)	27.76 – 2.20 26.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.76-2.20) 99.6 (26.77-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0095	Depositor
R, $R_{free}$	0.197 , 0.249 0.220 , 0.263	Depositor DCC
$R_{free}$ test set	3035 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.0	EDS
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60083 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 3PG

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	0.76	0/2563	0.79	2/3472 (0.1%)
1	P	0.79	0/2563	0.80	1/3473 (0.0%)
1	Q	0.84	0/2563	0.82	2/3472 (0.1%)
1	R	0.83	0/2561	0.85	3/3470 (0.1%)
All	All	0.81	0/10250	0.81	8/13887 (0.1%)

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	R	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	188	ASP	CB-CG-OD1	9.46	126.82	118.30
1	Q	188	ASP	CB-CG-OD1	8.09	125.58	118.30
1	O	15	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	R	293	ASP	CB-CG-OD1	7.15	124.74	118.30
1	P	15	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	R	293	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	O	188	ASP	CB-CG-OD1	5.80	123.52	118.30
1	Q	200	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	177	ILE	Peptide

## 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	2529	0	2510	43	0
1	P	2526	0	2502	49	0
1	Q	2529	0	2510	48	0
1	R	2527	0	2503	39	0
2	O	11	0	4	0	0
2	P	11	0	4	0	0
2	Q	11	0	4	0	0
2	R	11	0	4	1	0
3	O	44	0	26	1	0
3	P	44	0	26	3	0
3	Q	44	0	26	1	0
3	R	44	0	26	0	0
4	O	73	0	0	10	0
4	P	62	0	0	5	0
4	Q	60	0	0	9	0
4	R	68	0	0	9	0
All	All	10594	0	10145	155	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 8.

All (155) 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:265:ASN:HB3	4:O:400:HOH:O	1.34	1.25
1:Q:55:THR:HA	4:Q:356:HOH:O	1.45	1.14
1:O:269:GLU:HG2	4:O:406:HOH:O	1.55	1.03
1:R:265:ASN:HB3	4:R:373:HOH:O	1.56	1.02
1:R:198:ARG:HD3	4:R:381:HOH:O	1.60	1.00
1:Q:133:ASN:H	1:Q:136:HIS:CD2	1.81	0.98
1:Q:159:VAL:HA	4:Q:383:HOH:O	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:133:ASN:H	1:R:136:HIS:HD2	1.04	0.96
1:O:133:ASN:H	1:O:136:HIS:HD2	1.12	0.95
1:R:133:ASN:H	1:R:136:HIS:CD2	1.84	0.95
1:P:133:ASN:H	1:P:136:HIS:CD2	1.85	0.95
1:Q:133:ASN:H	1:Q:136:HIS:HD2	0.97	0.94
1:P:133:ASN:H	1:P:136:HIS:HD2	1.04	0.93
1:Q:245:LEU:HB2	4:Q:387:HOH:O	1.71	0.90
1:O:133:ASN:H	1:O:136:HIS:CD2	1.92	0.87
1:P:3:VAL:HG21	1:P:332:ALA:HB1	1.58	0.84
1:Q:263:MET:SD	4:Q:383:HOH:O	2.41	0.79
1:Q:3:VAL:HG21	1:Q:332:ALA:HB1	1.64	0.78
1:Q:133:ASN:N	1:Q:136:HIS:HD2	1.79	0.77
1:P:183[B]:ASP:OD2	1:P:198:ARG:NH1	2.18	0.76
1:R:3:VAL:HG21	1:R:332:ALA:HB1	1.68	0.75
1:O:3:VAL:HG21	1:O:332:ALA:HB1	1.68	0.74
1:O:192:ARG:NE	4:O:408:HOH:O	2.20	0.73
1:P:73:LYS:HE2	4:P:379:HOH:O	1.89	0.72
1:R:133:ASN:N	1:R:136:HIS:HD2	1.84	0.72
1:Q:115:LYS:HE2	4:Q:384:HOH:O	1.91	0.70
1:O:192:ARG:CB	4:O:409:HOH:O	2.42	0.67
1:O:309:LYS:HE3	4:O:369:HOH:O	1.99	0.63
1:O:133:ASN:N	1:O:136:HIS:HD2	1.91	0.61
1:O:192:ARG:HB2	4:O:409:HOH:O	2.00	0.61
1:P:133:ASN:N	1:P:136:HIS:HD2	1.87	0.61
1:R:104:ASP:O	1:R:107:GLN:HB3	2.00	0.60
1:Q:57:GLU:H	1:Q:68:ASN:ND2	2.00	0.60
1:P:205:ASN:HD22	1:O:281:SER:H	1.50	0.57
1:O:3:VAL:HB	1:O:27:LEU:HD23	1.87	0.57
1:O:309:LYS:CE	4:O:369:HOH:O	2.53	0.57
1:P:300:MET:CE	1:P:302:VAL:HG23	2.35	0.57
1:P:57:GLU:H	1:P:68:ASN:ND2	2.04	0.56
1:Q:205:ASN:HD22	1:R:281:SER:H	1.54	0.55
1:P:233:GLN:HE22	1:O:296:GLN:HE22	1.54	0.54
1:P:83:LEU:HD13	1:P:85:TRP:CZ2	2.42	0.54
1:P:307:LEU:HD21	1:O:307:LEU:HD21	1.90	0.53
1:P:53:ARG:HG3	4:R:370:HOH:O	2.07	0.53
1:Q:196:LYS:HB3	1:P:43:HIS:CD2	2.43	0.53
1:Q:34:ASP:O	1:Q:76:SER:HA	2.09	0.53
1:O:57:GLU:H	1:O:68:ASN:ND2	2.07	0.53
1:Q:11:GLY:HA3	3:Q:337:NAD:O5B	2.09	0.53
1:R:19:ARG:HD3	4:R:351:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:315:ASP:O	1:P:319:SER:HB2	2.09	0.52
1:P:205:ASN:ND2	1:O:281:SER:H	2.07	0.51
1:R:57:GLU:H	1:R:68:ASN:ND2	2.08	0.51
1:P:11:GLY:HA3	3:P:337:NAD:O5B	2.10	0.51
1:O:316:ASN:O	3:O:337:NAD:H4N	2.10	0.50
1:P:300:MET:CE	1:P:302:VAL:CG2	2.89	0.50
1:O:16:LEU:HD21	1:O:51:GLN:HG3	1.94	0.50
1:Q:32:VAL:O	1:Q:74:SER:HA	2.12	0.50
1:P:283:VAL:O	1:P:315:ASP:HB2	2.12	0.50
1:P:133:ASN:N	1:P:136:HIS:CD2	2.68	0.50
1:Q:43:HIS:CG	1:P:196:LYS:HD2	2.47	0.49
1:Q:298:ARG:NH2	4:Q:390:HOH:O	2.45	0.49
1:R:155:SER:HA	1:R:290:SER:HB2	1.94	0.49
1:O:300:MET:HE3	1:O:302:VAL:HG23	1.94	0.49
1:Q:57:GLU:H	1:Q:68:ASN:HD21	1.59	0.49
1:O:34:ASP:O	1:O:76:SER:HA	2.12	0.49
4:P:348:HOH:O	1:R:53:ARG:HD2	2.13	0.48
1:Q:300:MET:CE	1:Q:302:VAL:HG23	2.42	0.48
1:O:243:THR:O	1:O:311:ALA:HA	2.14	0.48
1:Q:300:MET:HE2	1:Q:302:VAL:HG23	1.94	0.48
1:P:12:ARG:HH11	1:P:15:ARG:NH2	2.11	0.48
1:P:316:ASN:OD1	3:P:337:NAD:N7N	2.45	0.48
1:P:279:VAL:HG23	1:O:205:ASN:ND2	2.28	0.48
1:O:181:THR:OG1	1:O:183:ASP:OD2	2.26	0.48
1:Q:184:GLN:HB3	4:Q:340:HOH:O	2.14	0.48
1:Q:283:VAL:O	1:Q:315:ASP:HB2	2.14	0.47
1:Q:300:MET:CE	1:Q:302:VAL:CG2	2.91	0.47
1:P:39:ASP:HB2	4:P:394:HOH:O	2.14	0.47
1:R:265:ASN:ND2	4:R:354:HOH:O	2.48	0.47
1:Q:307:LEU:HD21	1:R:307:LEU:HD21	1.96	0.47
1:P:211:THR:HG22	1:P:231:GLY:HA2	1.97	0.47
1:R:12:ARG:HH11	1:R:15:ARG:NH2	2.12	0.47
1:R:122:PRO:HD3	1:R:150:SER:HB3	1.97	0.47
1:P:300:MET:HE3	1:P:302:VAL:HG23	1.96	0.47
1:Q:196:LYS:HD2	1:P:43:HIS:CG	2.50	0.47
1:R:95:GLU:HG3	4:R:361:HOH:O	2.14	0.46
1:P:181:THR:OG1	1:P:183[A]:ASP:OD2	2.26	0.46
1:R:263:MET:HG3	1:R:292:PHE:CE1	2.50	0.46
1:O:273:TYR:HB2	4:O:360:HOH:O	2.14	0.46
1:O:15:ARG:NH2	4:O:339:HOH:O	2.39	0.46
1:R:92:VAL:HG11	1:R:328:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:103:LYS:HB2	1:Q:127:LEU:HD23	1.97	0.46
1:R:133:ASN:N	1:R:136:HIS:CD2	2.68	0.46
1:P:49:THR:HA	1:R:281:SER:OG	2.16	0.46
1:O:265:ASN:CB	4:O:400:HOH:O	2.20	0.45
2:R:338:3PG:C1	4:R:406:HOH:O	2.65	0.45
1:R:300:MET:HE3	1:R:302:VAL:HG23	1.99	0.45
1:R:283:VAL:O	1:R:315:ASP:HB2	2.16	0.45
1:R:3:VAL:HB	1:R:27:LEU:HD23	1.98	0.45
1:Q:205:ASN:ND2	1:R:279:VAL:HG23	2.31	0.45
1:P:278:ILE:HD11	1:P:313:TRP:CD1	2.51	0.45
1:P:243:THR:O	1:P:311:ALA:HA	2.17	0.45
1:P:3:VAL:HB	1:P:27:LEU:HD23	1.98	0.45
1:O:104:ASP:O	1:O:107:GLN:HB3	2.17	0.45
1:Q:281:SER:H	1:R:205:ASN:HD22	1.65	0.45
1:R:243:THR:O	1:R:311:ALA:HA	2.17	0.44
1:O:300:MET:CE	1:O:302:VAL:HG23	2.48	0.44
1:Q:222:PRO:HG3	4:Q:365:HOH:O	2.18	0.44
1:P:263:MET:HG3	1:P:292:PHE:CE1	2.52	0.44
1:P:184:GLN:HB3	4:P:341:HOH:O	2.16	0.44
1:Q:49:THR:HA	1:O:281:SER:OG	2.18	0.44
1:O:57:GLU:H	1:O:68:ASN:HD21	1.66	0.44
1:Q:205:ASN:ND2	1:R:281:SER:H	2.14	0.44
1:P:263:MET:HG3	1:P:292:PHE:CZ	2.53	0.43
1:Q:95:GLU:HB3	1:Q:119:ILE:HA	2.00	0.43
1:P:57:GLU:H	1:P:68:ASN:HD21	1.67	0.43
1:P:226:GLY:O	1:O:300:MET:HE1	2.18	0.43
1:P:316:ASN:HB2	3:P:337:NAD:H71N	1.83	0.43
1:Q:243:THR:O	1:Q:311:ALA:HA	2.19	0.43
1:Q:188:ASP:OD1	1:P:49:THR:OG1	2.29	0.43
1:R:245:LEU:HG	1:R:247:VAL:HG13	1.99	0.43
1:O:283:VAL:O	1:O:315:ASP:HB2	2.18	0.43
1:R:110:ILE:HD11	1:R:117:VAL:HG23	1.99	0.43
1:R:263:MET:HG3	1:R:292:PHE:CZ	2.54	0.43
1:O:263:MET:HG3	1:O:292:PHE:CZ	2.54	0.43
1:P:205:ASN:HD21	1:O:281:SER:CB	2.32	0.43
1:O:92:VAL:HG11	1:O:328:LEU:CD1	2.48	0.42
1:Q:300:MET:O	1:Q:306:GLN:HA	2.19	0.42
1:Q:233:GLN:HE22	1:R:296:GLN:HE22	1.67	0.42
1:P:92:VAL:HG11	1:P:328:LEU:CD1	2.49	0.42
1:P:300:MET:O	1:P:306:GLN:HA	2.20	0.42
1:P:281:SER:H	1:O:205:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:12:ARG:HH11	1:O:15:ARG:NH2	2.17	0.42
1:Q:80:ALA:HA	1:Q:83:LEU:HD12	2.02	0.42
1:Q:83:LEU:HD13	1:Q:85:TRP:CZ2	2.54	0.41
1:P:296:GLN:HE22	1:O:233:GLN:HE22	1.67	0.41
1:R:261:GLU:HG3	4:R:354:HOH:O	2.20	0.41
1:Q:228:LEU:HD22	1:Q:245:LEU:HD11	2.03	0.41
1:Q:240:GLY:H	1:Q:316:ASN:ND2	2.19	0.41
1:P:206:ILE:HB	1:O:280:SER:HB3	2.02	0.41
1:O:315:ASP:CG	1:O:318:MET:H	2.23	0.41
1:Q:240:GLY:H	1:Q:316:ASN:HD21	1.69	0.41
1:R:34:ASP:OD2	1:R:35:LEU:N	2.43	0.41
1:R:85:TRP:CE3	1:R:85:TRP:HA	2.56	0.41
1:Q:263:MET:HG3	1:Q:292:PHE:CZ	2.55	0.41
1:Q:3:VAL:HB	1:Q:27:LEU:HD23	2.03	0.41
1:Q:226:GLY:O	1:R:300:MET:HE1	2.20	0.41
1:Q:281:SER:OG	1:O:49:THR:HA	2.21	0.41
1:O:189:ALA:O	1:O:199:ALA:HB1	2.21	0.41
1:P:82:LYS:HD3	4:P:361:HOH:O	2.21	0.41
1:Q:300:MET:HE2	1:Q:302:VAL:CG2	2.51	0.41
1:P:242:LEU:HD13	1:P:313:TRP:CD2	2.56	0.41
1:Q:243:THR:HG22	4:Q:387:HOH:O	2.21	0.40
1:R:309:LYS:HE3	4:R:345:HOH:O	2.21	0.40
1:Q:296:GLN:HE22	1:R:233:GLN:HE22	1.69	0.40
1:R:85:TRP:HE3	1:R:85:TRP:HA	1.86	0.40
1:P:169:LEU:HD21	1:P:228:LEU:HD21	2.03	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%)	316 (95%)	15 (4%)	1 (0%)	46 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	332/336 (99%)	315 (95%)	16 (5%)	1 (0%)	46	50
1	Q	332/336 (99%)	311 (94%)	20 (6%)	1 (0%)	46	50
1	R	332/336 (99%)	313 (94%)	19 (6%)	0	100	100
All	All	1328/1344 (99%)	1255 (94%)	70 (5%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	62	ASP
1	P	62	ASP
1	Q	62	ASP

### 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	271/273 (99%)	263 (97%)	8 (3%)	48	60
1	P	271/273 (99%)	263 (97%)	8 (3%)	48	60
1	Q	271/273 (99%)	265 (98%)	6 (2%)	60	72
1	R	271/273 (99%)	262 (97%)	9 (3%)	45	56
All	All	1084/1092 (99%)	1053 (97%)	31 (3%)	50	62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	32	VAL
1	Q	39	ASP
1	Q	62	ASP
1	Q	85	TRP
1	Q	87	ASP
1	Q	253	ASP
1	P	32	VAL
1	P	39	ASP

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Mol	Chain	Res	Type
1	P	62	ASP
1	P	85	TRP
1	P	87	ASP
1	P	186	THR
1	P	253	ASP
1	P	269	GLU
1	O	32	VAL
1	O	39	ASP
1	O	62	ASP
1	O	76	SER
1	O	85	TRP
1	O	186	THR
1	O	239	THR
1	O	253	ASP
1	R	25	GLU
1	R	32	VAL
1	R	35	LEU
1	R	39	ASP
1	R	62	ASP
1	R	76	SER
1	R	85	TRP
1	R	239	THR
1	R	253	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	68	ASN
1	Q	136	HIS
1	Q	205	ASN
1	Q	265	ASN
1	Q	296	GLN
1	Q	316	ASN
1	P	68	ASN
1	P	136	HIS
1	P	205	ASN
1	P	265	ASN
1	P	296	GLN
1	O	68	ASN
1	O	136	HIS
1	O	205	ASN
1	O	265	ASN

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Mol	Chain	Res	Type
1	O	296	GLN
1	R	68	ASN
1	R	136	HIS
1	R	205	ASN
1	R	209	ASN
1	R	265	ASN
1	R	296	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	O	337	-	38,48,48	1.78	6 (15%)	47,73,73	2.62	14 (29%)
2	3PG	O	338	-	7,10,10	0.74	0	7,14,14	1.83	3 (42%)
3	NAD	P	337	-	38,48,48	1.58	2 (5%)	47,73,73	2.75	11 (23%)
2	3PG	P	338	-	7,10,10	0.67	0	7,14,14	1.71	1 (14%)
3	NAD	Q	337	-	38,48,48	1.45	4 (10%)	47,73,73	2.27	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3PG	Q	338	-	7,10,10	0.75	0	7,14,14	1.96	3 (42%)
3	NAD	R	337	-	38,48,48	1.96	5 (13%)	47,73,73	2.30	10 (21%)
2	3PG	R	338	-	7,10,10	0.90	0	7,14,14	2.21	3 (42%)

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	337	-	-	0/22/62/62	0/5/5/5
2	3PG	O	338	-	-	0/6/10/10	0/0/0/0
3	NAD	P	337	-	-	0/22/62/62	0/5/5/5
2	3PG	P	338	-	-	0/6/10/10	0/0/0/0
3	NAD	Q	337	-	-	0/22/62/62	0/5/5/5
2	3PG	Q	338	-	-	0/6/10/10	0/0/0/0
3	NAD	R	337	-	-	0/22/62/62	0/5/5/5
2	3PG	R	338	-	-	0/6/10/10	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	337	NAD	O4B-C4B	-2.33	1.39	1.45
3	O	337	NAD	PN-O1N	-2.27	1.42	1.51
3	O	337	NAD	PA-O2A	-2.18	1.45	1.54
3	O	337	NAD	C2A-N1A	2.22	1.38	1.33
3	Q	337	NAD	C2A-N1A	2.28	1.38	1.33
3	R	337	NAD	C8A-N7A	2.52	1.39	1.34
3	R	337	NAD	C2A-N1A	2.57	1.38	1.33
3	R	337	NAD	C2N-C3N	2.87	1.43	1.39
3	P	337	NAD	C2A-N3A	2.97	1.37	1.32
3	Q	337	NAD	C7N-N7N	3.33	1.39	1.33
3	O	337	NAD	C2A-N3A	3.81	1.38	1.32
3	Q	337	NAD	C2A-N3A	4.38	1.39	1.32
3	Q	337	NAD	O7N-C7N	4.49	1.33	1.24
3	R	337	NAD	C2A-N3A	4.61	1.40	1.32
3	P	337	NAD	O7N-C7N	7.47	1.40	1.24
3	O	337	NAD	O7N-C7N	8.02	1.41	1.24
3	R	337	NAD	O7N-C7N	9.12	1.43	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	337	NAD	N3A-C2A-N1A	-13.99	118.18	128.89
3	Q	337	NAD	N3A-C2A-N1A	-13.03	118.92	128.89
3	R	337	NAD	N3A-C2A-N1A	-10.15	121.12	128.89
3	O	337	NAD	N3A-C2A-N1A	-9.19	121.86	128.89
3	P	337	NAD	O3-PN-O5D	-5.75	87.67	102.94
3	R	337	NAD	C4A-C5A-N7A	-4.55	105.29	109.48
3	P	337	NAD	C1B-N9A-C4A	-4.39	120.32	126.94
3	O	337	NAD	C4A-C5A-N7A	-4.25	105.57	109.48
3	O	337	NAD	PN-O3-PA	-3.92	121.73	132.73
3	O	337	NAD	O7N-C7N-C3N	-3.83	115.40	119.59
2	R	338	3PG	O4P-P-O1P	-3.53	96.41	106.56
3	R	337	NAD	C1B-N9A-C4A	-3.47	121.71	126.94
3	O	337	NAD	C5N-C4N-C3N	-3.45	116.00	120.33
3	P	337	NAD	PN-O3-PA	-3.01	124.28	132.73
3	R	337	NAD	O3-PN-O5D	-2.98	95.04	102.94
2	O	338	3PG	O3-C2-C1	-2.96	102.37	111.44
3	O	337	NAD	O3D-C3D-C4D	-2.87	102.43	111.05
3	R	337	NAD	O3B-C3B-C4B	-2.86	102.47	111.05
2	O	338	3PG	O4P-P-O1P	-2.85	98.36	106.56
3	R	337	NAD	C4N-C3N-C7N	-2.79	113.71	121.09
3	O	337	NAD	O4B-C1B-N9A	-2.60	102.66	108.10
2	P	338	3PG	O4P-P-O1P	-2.57	99.16	106.56
3	P	337	NAD	O4B-C1B-N9A	-2.51	102.84	108.10
3	R	337	NAD	O3-PA-O5B	-2.42	96.52	102.94
3	P	337	NAD	O7N-C7N-N7N	-2.28	119.39	122.59
2	Q	338	3PG	O1P-P-O2P	-2.28	101.34	107.14
2	Q	338	3PG	O3-C2-C1	-2.22	104.64	111.44
3	Q	337	NAD	C4B-O4B-C1B	-2.19	107.32	109.72
2	R	338	3PG	O1P-P-O2P	-2.17	101.61	107.14
2	O	338	3PG	O4P-P-O3P	2.03	115.13	107.38
3	O	337	NAD	C3N-C7N-N7N	2.26	120.29	117.82
3	R	337	NAD	C2N-C3N-C4N	2.37	120.93	118.29
3	P	337	NAD	C2A-N1A-C6A	2.41	123.07	118.77
3	R	337	NAD	O2N-PN-O3	2.47	116.31	105.09
3	P	337	NAD	C4D-O4D-C1D	2.78	112.78	109.72
3	O	337	NAD	O2A-PA-O3	3.25	119.83	105.09
3	P	337	NAD	C2B-C1B-N9A	3.28	119.31	114.29
3	O	337	NAD	C2N-C3N-C4N	3.30	121.96	118.29
3	O	337	NAD	C4B-O4B-C1B	3.44	113.49	109.72
2	Q	338	3PG	O4P-P-O2P	3.50	121.83	110.58
3	O	337	NAD	C2B-C1B-N9A	3.51	119.65	114.29
2	R	338	3PG	O3P-P-O2P	3.53	121.95	110.58
3	P	337	NAD	O4D-C1D-N1N	4.12	112.66	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	R	337	NAD	O4D-C1D-N1N	4.32	112.88	108.13
3	P	337	NAD	C3N-C7N-N7N	4.33	122.56	117.82
3	Q	337	NAD	O4D-C1D-N1N	4.52	113.10	108.13
3	O	337	NAD	C4D-O4D-C1D	4.61	114.78	109.72
3	O	337	NAD	O4D-C1D-N1N	8.01	116.93	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	337	NAD	1	0
3	P	337	NAD	3	0
3	Q	337	NAD	1	0
2	R	338	3PG	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 ⓘ

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	334/336 (99%)	0.51	29 (8%) 13 12	28, 45, 68, 78	0
1	P	333/336 (99%)	0.52	33 (9%) 9 8	27, 44, 67, 75	0
1	Q	334/336 (99%)	0.37	24 (7%) 18 18	27, 44, 65, 80	0
1	R	334/336 (99%)	0.53	32 (9%) 10 9	27, 45, 73, 91	0
All	All	1335/1344 (99%)	0.48	118 (8%) 12 11	27, 44, 69, 91	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	192	ARG	6.0
1	R	63	GLY	5.7
1	O	193	LYS	5.4
1	P	192	ARG	5.3
1	O	94	LEU	5.1
1	Q	1	MET	5.0
1	P	94	LEU	4.6
1	Q	137	GLN	4.6
1	P	7	ILE	4.5
1	Q	192	ARG	4.5
1	O	66	ARG	4.2
1	O	304	ASP	4.2
1	O	192	ARG	4.2
1	R	89	ASN	4.0
1	O	302	VAL	3.9
1	R	87	ASP	3.9
1	R	214	ALA	3.8
1	Q	334	LEU	3.8
1	P	17	ALA	3.7
1	Q	57	GLU	3.7
1	O	7	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	R	304	ASP	3.5
1	P	2	ALA	3.5
1	P	55	THR	3.5
1	Q	141	GLY	3.5
1	O	69	GLY	3.5
1	R	88	LEU	3.5
1	R	7	ILE	3.4
1	R	62	ASP	3.4
1	P	87	ASP	3.3
1	R	25	GLU	3.2
1	R	335	SER	3.2
1	R	14	GLY	3.1
1	P	99	PHE	3.1
1	R	2	ALA	3.0
1	O	107	GLN	3.0
1	Q	94	LEU	3.0
1	O	334	LEU	3.0
1	R	215	LYS	3.0
1	O	59	GLU	3.0
1	O	324	LEU	3.0
1	P	32	VAL	2.9
1	Q	14	GLY	2.9
1	R	13	ILE	2.9
1	O	62	ASP	2.9
1	O	1	MET	2.9
1	R	82	LYS	2.9
1	O	5	VAL	2.8
1	R	193	LYS	2.8
1	Q	252	GLN	2.7
1	R	265	ASN	2.7
1	O	137	GLN	2.7
1	R	99	PHE	2.7
1	Q	55	THR	2.7
1	O	55	THR	2.7
1	O	70	LYS	2.7
1	P	304	ASP	2.7
1	P	252	GLN	2.6
1	R	86	LYS	2.6
1	R	10	PHE	2.6
1	P	245	LEU	2.6
1	O	243	THR	2.6
1	P	16	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	13	ILE	2.5
1	O	99	PHE	2.5
1	O	93	VAL	2.5
1	P	63	GLY	2.5
1	Q	59	GLU	2.5
1	O	32	VAL	2.5
1	O	61	VAL	2.5
1	Q	126	ASP	2.5
1	R	252	GLN	2.5
1	R	216	ALA	2.5
1	R	69	GLY	2.5
1	P	62	ASP	2.5
1	Q	125	GLY	2.4
1	O	246	THR	2.4
1	Q	7	ILE	2.4
1	Q	66	ARG	2.4
1	O	126	ASP	2.4
1	R	39	ASP	2.4
1	Q	2	ALA	2.4
1	P	324	LEU	2.4
1	R	66	ARG	2.4
1	Q	304	ASP	2.3
1	O	253	ASP	2.3
1	Q	10	PHE	2.3
1	P	246	THR	2.3
1	P	66	ARG	2.3
1	Q	13	ILE	2.3
1	P	14	GLY	2.3
1	R	16	LEU	2.3
1	O	252	GLN	2.3
1	R	64	GLY	2.3
1	P	10	PHE	2.3
1	P	73	LYS	2.3
1	R	324	LEU	2.3
1	P	334	LEU	2.2
1	P	107	GLN	2.2
1	Q	86	LYS	2.2
1	P	57	GLU	2.2
1	R	111	GLU	2.2
1	P	68	ASN	2.2
1	P	5	VAL	2.2
1	Q	9	GLY	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	P	194	GLY	2.1
1	O	14	GLY	2.1
1	O	111	GLU	2.1
1	P	320	TYR	2.1
1	Q	81	SER	2.1
1	P	137	GLN	2.1
1	Q	173	LEU	2.1
1	P	93	VAL	2.1
1	Q	330	TYR	2.0
1	R	73	LYS	2.0
1	P	6	ALA	2.0
1	P	108	ALA	2.0
1	R	94	LEU	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
2	3PG	R	338	11/11	0.93	0.18	1.04	22,44,53,57	0
3	NAD	Q	337	44/44	0.96	0.12	-0.98	29,37,48,50	0
2	3PG	Q	338	11/11	0.96	0.10	-1.11	27,36,45,47	0
3	NAD	R	337	44/44	0.95	0.10	-1.45	8,20,29,31	0
3	NAD	P	337	44/44	0.96	0.09	-1.49	12,19,25,28	0
2	3PG	P	338	11/11	0.97	0.10	-1.59	25,37,41,43	0
3	NAD	O	337	44/44	0.95	0.10	-1.61	8,20,27,30	0
2	3PG	O	338	11/11	0.97	0.10	-1.62	22,33,42,44	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.