



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:20 am GMT

PDB ID : 2B4R  
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from Plasmodium falciparum at 2.25 Angstrom Resolution reveals intriguing extra electron density in the active site  
Authors : Robien, M.A.; Bosch, J.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)  
Deposited on : 2005-09-26  
Resolution : 2.25 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

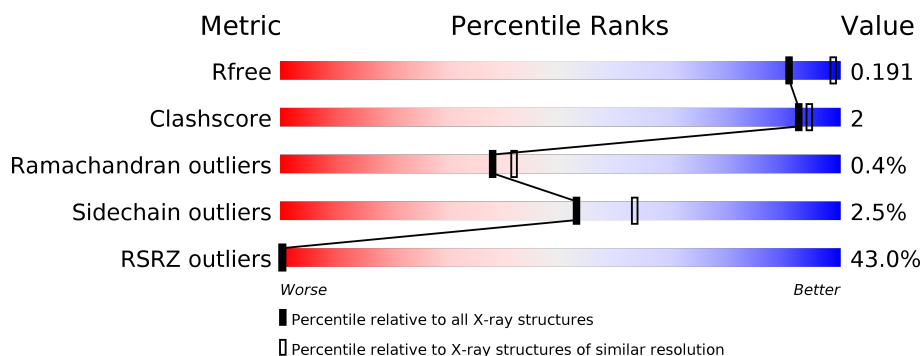
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	345	<div> <div>45%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	P	345	<div> <div>43%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	Q	345	<div> <div>43%</div> <div>90%</div> <div>6%</div> <div>..</div> </div>
1	R	345	<div> <div>36%</div> <div>87%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10700 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	58	0	0
			2551	1627	438	473	13			
1	P	334	Total	C	N	O	S	73	0	0
			2551	1627	438	473	13			
1	Q	334	Total	C	N	O	S	57	0	0
			2551	1627	438	473	13			
1	R	334	Total	C	N	O	S	47	0	0
			2551	1627	438	473	13			

There are 44 discrepancies between the modelled and reference sequences:

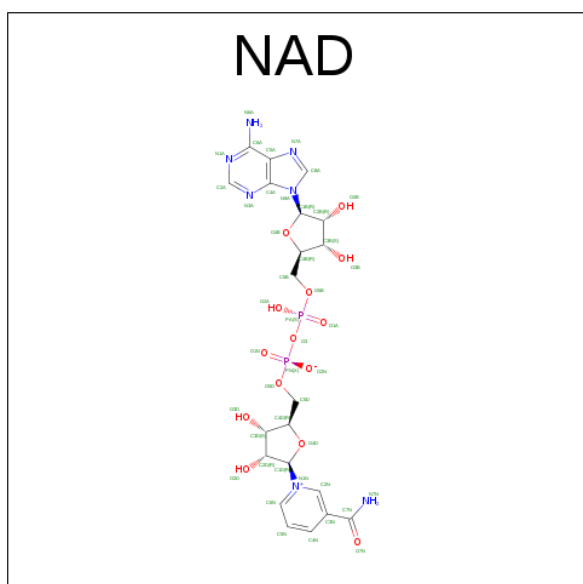
Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
O	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
O	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-1	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	0	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	3	ALA	VAL	ENGINEERED	UNP Q8T6B1
O	336	THR	ASN	ENGINEERED	UNP Q8T6B1
O	337	SER	ASN	ENGINEERED	UNP Q8T6B1
P	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
P	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
P	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
P	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
P	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
P	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
P	-1	HIS	-	EXPRESSION TAG	UNP Q8T6B1
P	0	HIS	-	EXPRESSION TAG	UNP Q8T6B1
P	3	ALA	VAL	ENGINEERED	UNP Q8T6B1
P	336	THR	ASN	ENGINEERED	UNP Q8T6B1

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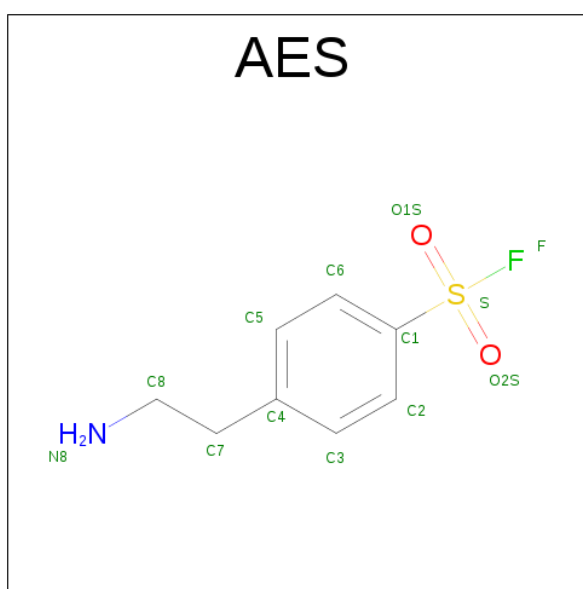
Chain	Residue	Modelled	Actual	Comment	Reference
P	337	SER	ASN	ENGINEERED	UNP Q8T6B1
Q	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-1	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	0	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	3	ALA	VAL	ENGINEERED	UNP Q8T6B1
Q	336	THR	ASN	ENGINEERED	UNP Q8T6B1
Q	337	SER	ASN	ENGINEERED	UNP Q8T6B1
R	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
R	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
R	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
R	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
R	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
R	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
R	-1	HIS	-	EXPRESSION TAG	UNP Q8T6B1
R	0	HIS	-	EXPRESSION TAG	UNP Q8T6B1
R	3	ALA	VAL	ENGINEERED	UNP Q8T6B1
R	336	THR	ASN	ENGINEERED	UNP Q8T6B1
R	337	SER	ASN	ENGINEERED	UNP Q8T6B1

- 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	P	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	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (three-letter code: AES) (formula:  $C_8H_{10}FNO_2S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	O	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
3	P	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
3	R	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	R	1	Total	C	O	0	0
			6	3	3		
4	P	1	Total	C	O	0	0
			6	3	3		
4	O	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		

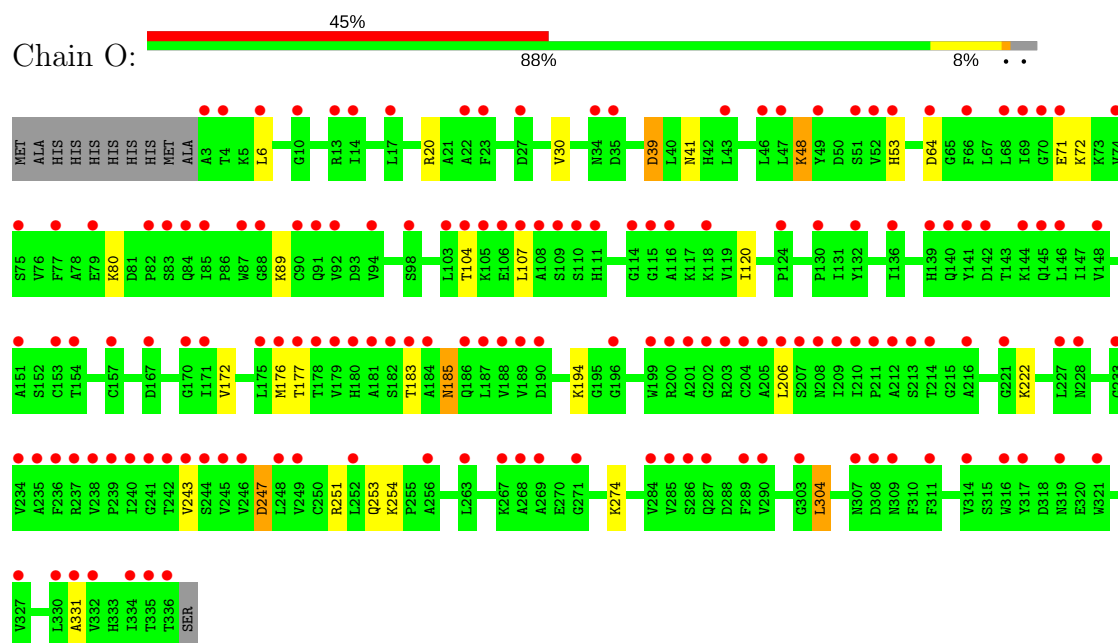
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	63	Total	O	0	0
			63	63		
5	P	67	Total	O	0	0
			67	67		
5	Q	53	Total	O	0	0
			53	53		
5	R	74	Total	O	0	0
			74	74		

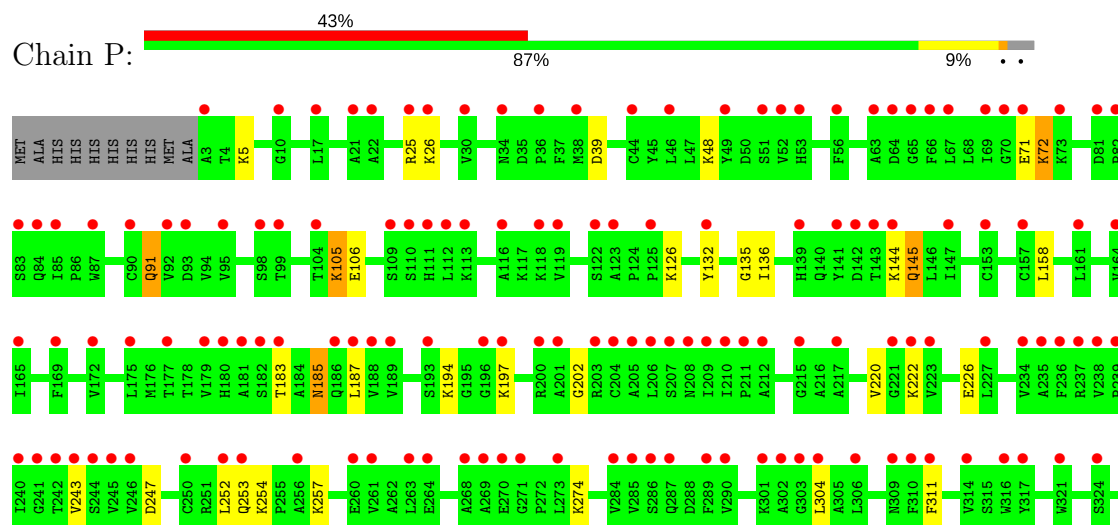
### 3 Residue-property plots [i](#)

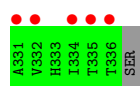
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase



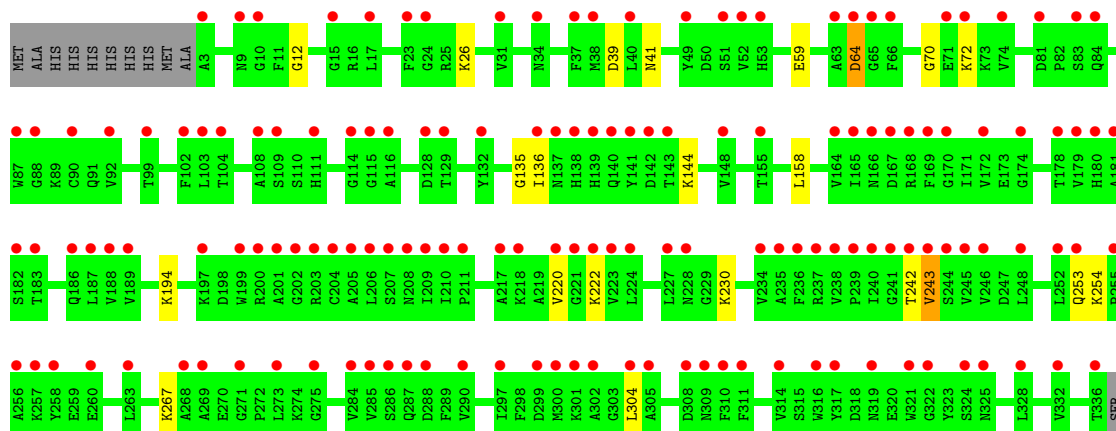
- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase





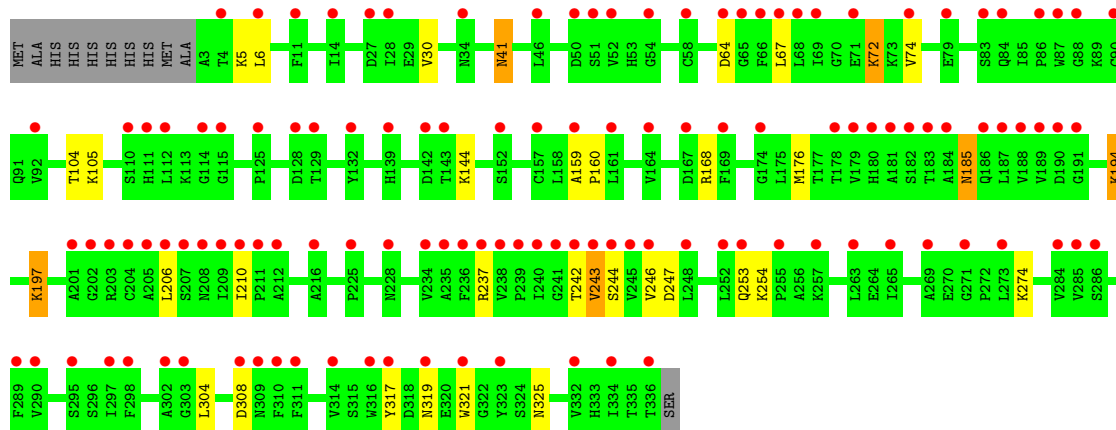
- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

Chain Q: 43% 90% 6% . .



- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

Chain R: 36% 87% 8% . .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.33Å 104.58Å 90.84Å 90.00° 107.35° 90.00°	Depositor
Resolution (Å)	46.37 – 2.25 46.36 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.37-2.25) 96.9 (46.36-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.243 0.193 , 0.191	Depositor DCC
$R_{free}$ test set	2861 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AES, 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	0.99	13/2603 (0.5%)	0.81	11/3528 (0.3%)
1	P	1.25	18/2603 (0.7%)	0.86	16/3528 (0.5%)
1	Q	0.92	11/2603 (0.4%)	0.92	14/3528 (0.4%)
1	R	0.77	9/2603 (0.3%)	0.74	11/3528 (0.3%)
All	All	1.00	51/10412 (0.5%)	0.84	52/14112 (0.4%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	71	GLU	CG-CD	-30.16	1.06	1.51
1	O	48	LYS	CD-CE	-24.67	0.89	1.51
1	P	253	GLN	CG-CD	-24.05	0.95	1.51
1	P	106	GLU	CG-CD	-22.93	1.17	1.51
1	O	247	ASP	CB-CG	-21.29	1.07	1.51
1	Q	253	GLN	CG-CD	-20.90	1.02	1.51
1	P	25	ARG	CG-CD	-19.54	1.03	1.51
1	P	105	LYS	CB-CG	-18.77	1.01	1.52
1	Q	267	LYS	CB-CG	-17.69	1.04	1.52
1	Q	72	LYS	CG-CD	-17.52	0.92	1.52
1	O	64	ASP	CA-CB	15.48	1.88	1.53
1	R	72	LYS	CG-CD	-15.39	1.00	1.52
1	Q	41	ASN	CB-CG	-14.99	1.16	1.51
1	O	254	LYS	CD-CE	-13.87	1.16	1.51
1	R	194	LYS	CB-CG	13.82	1.89	1.52
1	R	254	LYS	CB-CG	-12.68	1.18	1.52
1	R	144	LYS	CG-CD	-11.99	1.11	1.52
1	R	41	ASN	CB-CG	-11.81	1.23	1.51
1	O	194	LYS	CG-CD	-11.65	1.12	1.52
1	O	89	LYS	CD-CE	11.56	1.80	1.51
1	P	144	LYS	CD-CE	-11.25	1.23	1.51
1	Q	26	LYS	CB-CG	-11.20	1.22	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	48	LYS	CB-CG	-10.83	1.23	1.52
1	P	257	LYS	CG-CD	10.62	1.88	1.52
1	P	126	LYS	CD-CE	10.19	1.76	1.51
1	P	26	LYS	CB-CG	-10.18	1.25	1.52
1	Q	39	ASP	CB-CG	-9.34	1.32	1.51
1	O	72	LYS	CG-CD	9.14	1.83	1.52
1	Q	64	ASP	CA-CB	-9.01	1.34	1.53
1	P	91	GLN	CA-CB	-8.88	1.34	1.53
1	Q	254	LYS	CB-CG	-8.42	1.29	1.52
1	Q	144	LYS	CD-CE	8.27	1.72	1.51
1	R	5	LYS	CG-CD	-7.80	1.25	1.52
1	O	39	ASP	CB-CG	-7.65	1.35	1.51
1	O	71	GLU	CA-CB	-7.56	1.37	1.53
1	P	226	GLU	CG-CD	-7.34	1.41	1.51
1	O	41	ASN	CB-CG	-7.18	1.34	1.51
1	O	80	LYS	CB-CG	-7.11	1.33	1.52
1	O	274	LYS	CD-CE	-7.11	1.33	1.51
1	R	197	LYS	CB-CG	-7.11	1.33	1.52
1	Q	230	LYS	CD-CE	-6.68	1.34	1.51
1	R	254	LYS	CD-CE	6.62	1.67	1.51
1	P	72	LYS	CG-CD	-6.61	1.29	1.52
1	Q	194	LYS	CB-CG	-6.59	1.34	1.52
1	P	274	LYS	CG-CD	-6.47	1.30	1.52
1	R	274	LYS	CG-CD	-6.18	1.31	1.52
1	P	5	LYS	CB-CG	-6.09	1.36	1.52
1	P	254	LYS	CD-CE	6.07	1.66	1.51
1	P	194	LYS	CG-CD	-5.96	1.32	1.52
1	P	39	ASP	CB-CG	-5.29	1.40	1.51
1	O	253	GLN	CG-CD	-5.25	1.39	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	41	ASN	CA-CB-CG	20.48	158.45	113.40
1	Q	72	LYS	CB-CG-CD	18.86	160.64	111.60
1	P	72	LYS	CG-CD-CE	18.08	166.15	111.90
1	O	247	ASP	CB-CG-OD1	-15.35	104.48	118.30
1	Q	41	ASN	CB-CG-OD1	-14.96	91.67	121.60
1	R	253	GLN	CG-CD-OE1	-14.29	93.02	121.60
1	O	247	ASP	CB-CG-OD2	14.15	131.04	118.30
1	R	144	LYS	CB-CG-CD	12.75	144.75	111.60
1	Q	194	LYS	CA-CB-CG	12.59	141.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	247	ASP	CA-CB-CG	12.16	140.16	113.40
1	O	48	LYS	CG-CD-CE	11.80	147.30	111.90
1	Q	41	ASN	CB-CG-ND2	11.71	144.80	116.70
1	P	105	LYS	CA-CB-CG	11.27	138.19	113.40
1	O	194	LYS	CB-CG-CD	11.24	140.83	111.60
1	P	144	LYS	CD-CE-NZ	10.60	136.08	111.70
1	R	253	GLN	CG-CD-NE2	10.53	141.98	116.70
1	P	106	GLU	CB-CG-CD	10.40	142.28	114.20
1	O	80	LYS	CA-CB-CG	10.38	136.22	113.40
1	Q	64	ASP	CB-CA-C	10.17	130.75	110.40
1	Q	26	LYS	CB-CG-CD	10.00	137.60	111.60
1	R	72	LYS	CB-CG-CD	9.20	135.51	111.60
1	P	106	GLU	CG-CD-OE2	9.16	136.62	118.30
1	Q	72	LYS	CG-CD-CE	9.12	139.26	111.90
1	Q	26	LYS	CA-CB-CG	-9.03	93.53	113.40
1	P	253	GLN	CB-CG-CD	8.95	134.86	111.60
1	P	106	GLU	CG-CD-OE1	-8.64	101.02	118.30
1	P	71	GLU	CB-CG-CD	7.56	134.61	114.20
1	R	64	ASP	N-CA-CB	7.54	124.17	110.60
1	P	48	LYS	CA-CB-CG	7.41	129.70	113.40
1	Q	254	LYS	CA-CB-CG	7.39	129.66	113.40
1	P	71	GLU	CG-CD-OE2	7.34	132.99	118.30
1	R	72	LYS	CG-CD-CE	7.23	133.59	111.90
1	P	25	ARG	CB-CG-CD	6.92	129.59	111.60
1	P	71	GLU	CG-CD-OE1	-6.89	104.52	118.30
1	P	126	LYS	CG-CD-CE	-6.80	91.49	111.90
1	Q	267	LYS	CA-CB-CG	6.71	128.16	113.40
1	Q	194	LYS	CB-CG-CD	6.70	129.03	111.60
1	O	39	ASP	CB-CG-OD1	6.37	124.04	118.30
1	O	64	ASP	CB-CA-C	-6.27	97.86	110.40
1	P	26	LYS	CA-CB-CG	5.89	126.36	113.40
1	O	39	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	P	39	ASP	CB-CG-OD2	5.59	123.33	118.30
1	R	197	LYS	CA-CB-CG	5.55	125.60	113.40
1	O	274	LYS	CG-CD-CE	5.53	128.49	111.90
1	R	64	ASP	CB-CA-C	-5.48	99.44	110.40
1	Q	64	ASP	CA-CB-CG	5.40	125.28	113.40
1	P	226	GLU	CB-CG-CD	5.37	128.69	114.20
1	R	64	ASP	CA-CB-CG	-5.26	101.82	113.40
1	R	274	LYS	CB-CG-CD	5.21	125.16	111.60
1	Q	222	LYS	CB-CG-CD	5.19	125.10	111.60
1	O	253	GLN	CB-CG-CD	5.13	124.94	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	105	LYS	CD-CE-NZ	5.12	123.48	111.70

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	2551	0	2578	13	0
1	P	2551	0	2578	9	0
1	Q	2551	0	2578	4	0
1	R	2551	0	2578	13	0
2	O	44	0	26	0	0
2	P	44	0	26	0	0
2	Q	44	0	26	1	0
2	R	44	0	26	1	0
3	O	13	0	10	0	0
3	P	13	0	10	0	0
3	R	13	0	10	0	0
4	O	6	0	8	0	0
4	P	6	0	8	0	0
4	R	12	0	16	0	0
5	O	63	0	0	0	0
5	P	67	0	0	0	0
5	Q	53	0	0	0	0
5	R	74	0	0	0	0
All	All	10700	0	10478	37	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 2.

All (37) 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:185:ASN:H	1:P:185:ASN:HD22	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:185:ASN:H	1:R:185:ASN:HD22	1.38	0.69
1:P:183:THR:OG1	1:P:185:ASN:ND2	2.30	0.65
1:O:185:ASN:H	1:O:185:ASN:HD22	1.50	0.58
1:Q:158:LEU:HD23	1:Q:220:VAL:HG21	1.86	0.57
1:O:104:THR:HG22	1:O:107:LEU:HD12	1.86	0.56
1:O:185:ASN:HD22	1:O:185:ASN:N	2.03	0.56
1:P:158:LEU:HD23	1:P:220:VAL:HG21	1.88	0.56
1:O:183:THR:OG1	1:O:185:ASN:ND2	2.41	0.54
1:R:185:ASN:HD22	1:R:185:ASN:N	2.06	0.52
1:R:321:TRP:O	1:R:325:ASN:ND2	2.42	0.52
1:R:210:ILE:HB	1:R:237:ARG:HB2	1.93	0.51
1:R:176:MET:HG3	1:R:246:VAL:HG13	1.94	0.49
1:O:6:LEU:HD23	1:O:30:VAL:HG22	1.94	0.48
1:P:185:ASN:N	1:P:185:ASN:HD22	2.04	0.48
1:O:120:ILE:HD11	1:O:331:ALA:HA	1.97	0.47
1:O:177:THR:OG1	1:P:247:ASP:OD2	2.29	0.47
1:O:206:LEU:HG	1:R:206:LEU:HG	1.96	0.46
1:P:132:TYR:OH	1:P:145:GLN:OE1	2.14	0.46
1:Q:242:THR:HG23	1:Q:243:VAL:HG23	1.98	0.45
1:O:20:ARG:NH2	1:O:53:HIS:O	2.50	0.45
1:Q:12:GLY:HA3	2:Q:501:NAD:O5B	2.16	0.45
1:O:104:THR:HG23	1:O:107:LEU:H	1.82	0.45
1:R:6:LEU:HD23	1:R:30:VAL:HG22	1.99	0.45
1:R:244:SER:HB2	1:R:317:TYR:CZ	2.52	0.44
1:R:67:LEU:HB3	1:R:74:VAL:HB	1.99	0.44
1:P:187:LEU:HD12	1:P:202:GLY:HA2	2.01	0.43
1:R:159:ALA:HB3	1:R:160:PRO:HD3	1.99	0.43
1:P:135:GLY:C	1:P:136:ILE:HD12	2.40	0.42
1:O:206:LEU:N	1:O:206:LEU:HD12	2.35	0.41
1:R:206:LEU:HD12	1:R:206:LEU:N	2.35	0.41
1:R:242:THR:HG23	1:R:243:VAL:HG23	2.02	0.41
1:P:252:LEU:HD12	1:P:311:PHE:CE1	2.55	0.41
1:R:319:ASN:O	2:R:901:NAD:H4N	2.20	0.41
1:O:172:VAL:HG11	1:O:251:ARG:NH1	2.35	0.41
1:O:304:LEU:HD23	1:O:304:LEU:C	2.40	0.41
1:Q:135:GLY:C	1:Q:136:ILE:HD12	2.41	0.41

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	332/345 (96%)	314 (95%)	17 (5%)	1 (0%)	44	50
1	P	332/345 (96%)	314 (95%)	17 (5%)	1 (0%)	44	50
1	Q	332/345 (96%)	313 (94%)	17 (5%)	2 (1%)	28	29
1	R	332/345 (96%)	310 (93%)	21 (6%)	1 (0%)	44	50
All	All	1328/1380 (96%)	1251 (94%)	72 (5%)	5 (0%)	38	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	243	VAL
1	P	243	VAL
1	Q	243	VAL
1	R	243	VAL
1	Q	70	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	277/286 (97%)	270 (98%)	7 (2%)	53	63
1	P	277/286 (97%)	269 (97%)	8 (3%)	48	57
1	Q	277/286 (97%)	274 (99%)	3 (1%)	78	86
1	R	277/286 (97%)	267 (96%)	10 (4%)	40	49
All	All	1108/1144 (97%)	1080 (98%)	28 (2%)	53	63

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	39	ASP
1	O	48	LYS
1	O	176	MET
1	O	185	ASN
1	O	222	LYS
1	O	247	ASP
1	O	304	LEU
1	P	72	LYS
1	P	91	GLN
1	P	105	LYS
1	P	145	GLN
1	P	185	ASN
1	P	197	LYS
1	P	222	LYS
1	P	304	LEU
1	Q	59	GLU
1	Q	64	ASP
1	Q	304	LEU
1	R	41	ASN
1	R	72	LYS
1	R	104	THR
1	R	168	ARG
1	R	185	ASN
1	R	194	LYS
1	R	197	LYS
1	R	247	ASP
1	R	304	LEU
1	R	308	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	185	ASN
1	P	62	HIS
1	P	139	HIS
1	P	185	ASN
1	Q	139	HIS
1	R	138	HIS
1	R	185	ASN



### 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 ⓘ

11 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	AES	O	601	-	12,13,13	0.51	0	17,18,18	1.84	2 (11%)
2	NAD	O	801	-	41,48,48	1.59	3 (7%)	43,73,73	1.74	2 (4%)
4	GOL	O	804	-	5,5,5	0.32	0	5,5,5	0.22	0
3	AES	P	602	-	12,13,13	0.51	0	17,18,18	1.91	2 (11%)
2	NAD	P	701	-	41,48,48	1.60	3 (7%)	43,73,73	1.71	1 (2%)
4	GOL	P	703	-	5,5,5	0.35	0	5,5,5	0.27	0
2	NAD	Q	501	-	41,48,48	1.70	3 (7%)	43,73,73	1.81	1 (2%)
4	GOL	R	503	-	5,5,5	0.31	0	5,5,5	0.30	0
3	AES	R	603	-	12,13,13	0.50	0	17,18,18	1.87	2 (11%)
2	NAD	R	901	-	41,48,48	1.59	3 (7%)	43,73,73	1.84	3 (6%)
4	GOL	R	903	-	5,5,5	0.29	0	5,5,5	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
3	AES	O	601	-	-	0/9/9/9	0/1/1/1
2	NAD	O	801	-	-	0/22/62/62	0/5/5/5
4	GOL	O	804	-	-	0/4/4/4	0/0/0/0
3	AES	P	602	-	-	0/9/9/9	0/1/1/1
2	NAD	P	701	-	-	0/22/62/62	0/5/5/5
4	GOL	P	703	-	-	0/4/4/4	0/0/0/0
2	NAD	Q	501	-	-	0/22/62/62	0/5/5/5
4	GOL	R	503	-	-	0/4/4/4	0/0/0/0
3	AES	R	603	-	-	0/9/9/9	0/1/1/1
2	NAD	R	901	-	-	0/22/62/62	0/5/5/5
4	GOL	R	903	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	901	NAD	C2A-N1A	2.58	1.38	1.33
2	P	701	NAD	C2A-N1A	2.77	1.39	1.33
2	O	801	NAD	C2A-N1A	2.81	1.39	1.33
2	Q	501	NAD	C2A-N1A	2.84	1.39	1.33
2	P	701	NAD	C2A-N3A	3.84	1.38	1.32
2	Q	501	NAD	C2A-N3A	3.92	1.38	1.32
2	O	801	NAD	C2A-N3A	3.94	1.38	1.32
2	R	901	NAD	C2A-N3A	4.07	1.39	1.32
2	R	901	NAD	O7N-C7N	7.85	1.40	1.24
2	O	801	NAD	O7N-C7N	7.96	1.40	1.24
2	P	701	NAD	O7N-C7N	8.05	1.40	1.24
2	Q	501	NAD	O7N-C7N	8.73	1.42	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	501	NAD	N3A-C2A-N1A	-10.60	119.63	128.86
2	R	901	NAD	N3A-C2A-N1A	-10.44	119.77	128.86
2	O	801	NAD	N3A-C2A-N1A	-9.89	120.24	128.86
2	P	701	NAD	N3A-C2A-N1A	-9.86	120.27	128.86
3	P	602	AES	O2S-S-C1	-6.72	103.88	110.74
3	R	603	AES	O2S-S-C1	-5.83	104.79	110.74
3	O	601	AES	O2S-S-C1	-5.20	105.43	110.74
3	O	601	AES	O1S-S-C1	-4.89	105.75	110.74
3	R	603	AES	O1S-S-C1	-4.30	106.35	110.74
3	P	602	AES	O1S-S-C1	-2.85	107.83	110.74
2	R	901	NAD	C4A-C5A-N7A	-2.57	106.92	109.41
2	O	801	NAD	C4A-C5A-N7A	-2.34	107.15	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	901	NAD	C1B-N9A-C4A	-2.14	122.93	126.64

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	Q	501	NAD	1	0
2	R	901	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

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	334/345 (96%)	2.23	154 (46%) <b>0</b> <b>0</b>	57, 67, 80, 88	18 (5%)
1	P	334/345 (96%)	2.10	147 (44%) <b>0</b> <b>0</b>	51, 68, 84, 88	21 (6%)
1	Q	334/345 (96%)	2.17	150 (44%) <b>0</b> <b>0</b>	77, 88, 101, 114	17 (5%)
1	R	334/345 (96%)	1.89	123 (36%) <b>0</b> <b>0</b>	49, 61, 75, 89	14 (4%)
All	All	1336/1380 (96%)	2.10	574 (42%) <b>0</b> <b>0</b>	49, 69, 94, 114	70 (5%)

All (574) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	90	CYS	9.2
1	Q	217	ALA	9.1
1	P	206	LEU	8.4
1	O	85	ILE	8.1
1	R	206	LEU	7.7
1	P	209	ILE	7.3
1	Q	224	LEU	7.3
1	P	63	ALA	7.2
1	Q	206	LEU	7.1
1	O	240	ILE	7.0
1	Q	221	GLY	6.9
1	Q	209	ILE	6.7
1	O	209	ILE	6.6
1	O	206	LEU	6.6
1	Q	238	VAL	6.5
1	O	239	PRO	6.2
1	O	238	VAL	6.2
1	Q	99	THR	6.1
1	P	236	PHE	6.0
1	Q	240	ILE	6.0
1	O	92	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	R	87	TRP	6.0
1	R	114	GLY	6.0
1	O	205	ALA	5.9
1	O	210	ILE	5.8
1	O	82	PRO	5.8
1	P	84	GLN	5.7
1	P	69	ILE	5.7
1	P	240	ILE	5.7
1	R	238	VAL	5.7
1	P	66	PHE	5.7
1	Q	236	PHE	5.7
1	Q	116	ALA	5.7
1	R	52	VAL	5.5
1	O	336	THR	5.5
1	R	188	VAL	5.5
1	P	239	PRO	5.5
1	O	179	VAL	5.5
1	R	205	ALA	5.5
1	P	179	VAL	5.4
1	Q	205	ALA	5.4
1	Q	179	VAL	5.4
1	R	309	ASN	5.3
1	O	188	VAL	5.3
1	O	83	SER	5.3
1	R	209	ILE	5.3
1	O	241	GLY	5.2
1	P	241	GLY	5.2
1	R	207	SER	5.2
1	R	204	CYS	5.2
1	P	85	ILE	5.2
1	R	187	LEU	5.2
1	P	205	ALA	5.1
1	P	207	SER	5.1
1	R	240	ILE	5.1
1	Q	109	SER	5.0
1	P	238	VAL	5.0
1	P	83	SER	5.0
1	P	188	VAL	5.0
1	P	189	VAL	5.0
1	R	239	PRO	5.0
1	O	87	TRP	5.0
1	P	90	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	O	204	CYS	4.9
1	Q	239	PRO	4.9
1	P	52	VAL	4.9
1	O	6	LEU	4.9
1	O	236	PHE	4.9
1	O	75	SER	4.8
1	O	114	GLY	4.8
1	Q	285	VAL	4.8
1	R	179	VAL	4.8
1	O	207	SER	4.8
1	O	235	ALA	4.8
1	Q	207	SER	4.7
1	P	87	TRP	4.7
1	Q	227	LEU	4.7
1	R	90	CYS	4.7
1	Q	83	SER	4.7
1	O	187	LEU	4.7
1	R	184	ALA	4.6
1	P	196	GLY	4.6
1	R	65	GLY	4.6
1	O	116	ALA	4.6
1	O	245	VAL	4.6
1	Q	188	VAL	4.6
1	P	245	VAL	4.5
1	Q	143	THR	4.5
1	P	316	TRP	4.5
1	O	189	VAL	4.5
1	O	104	THR	4.4
1	Q	317	TYR	4.4
1	O	68	LEU	4.4
1	P	285	VAL	4.4
1	Q	204	CYS	4.4
1	O	91	GLN	4.4
1	P	210	ILE	4.4
1	P	187	LEU	4.4
1	O	52	VAL	4.4
1	O	94	VAL	4.4
1	R	241	GLY	4.3
1	Q	165	ILE	4.3
1	Q	242	THR	4.3
1	P	204	CYS	4.3
1	Q	210	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	O	22	ALA	4.3
1	O	234	VAL	4.3
1	Q	52	VAL	4.3
1	Q	316	TRP	4.3
1	O	182	SER	4.3
1	P	139	HIS	4.3
1	O	334	ILE	4.2
1	R	311	PHE	4.2
1	R	243	VAL	4.2
1	O	243	VAL	4.2
1	Q	245	VAL	4.2
1	O	252	LEU	4.2
1	Q	241	GLY	4.2
1	Q	290	VAL	4.2
1	Q	309	ASN	4.1
1	R	332	VAL	4.1
1	R	210	ILE	4.1
1	P	172	VAL	4.1
1	P	332	VAL	4.1
1	Q	253	GLN	4.1
1	O	10	GLY	4.0
1	Q	308	ASP	4.0
1	P	181	ALA	4.0
1	O	269	ALA	4.0
1	R	236	PHE	4.0
1	O	242	THR	4.0
1	P	242	THR	4.0
1	R	245	VAL	4.0
1	R	181	ALA	4.0
1	Q	170	GLY	3.9
1	Q	228	ASN	3.9
1	O	180	HIS	3.9
1	Q	142	ASP	3.9
1	Q	168	ARG	3.9
1	Q	141	TYR	3.9
1	Q	237	ARG	3.8
1	P	182	SER	3.8
1	O	79	GLU	3.8
1	P	208	ASN	3.8
1	Q	132	TYR	3.8
1	Q	311	PHE	3.8
1	R	186	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	Q	252	LEU	3.8
1	Q	208	ASN	3.8
1	R	285	VAL	3.7
1	Q	128	ASP	3.7
1	Q	189	VAL	3.7
1	P	311	PHE	3.7
1	P	243	VAL	3.7
1	O	237	ARG	3.7
1	O	308	ASP	3.6
1	P	25	ARG	3.6
1	P	273	LEU	3.6
1	Q	328	LEU	3.6
1	O	186	GLN	3.6
1	P	113	LYS	3.6
1	O	208	ASN	3.6
1	O	228	ASN	3.6
1	O	332	VAL	3.6
1	R	112	LEU	3.6
1	R	317	TYR	3.6
1	O	181	ALA	3.6
1	O	211	PRO	3.6
1	O	244	SER	3.6
1	Q	87	TRP	3.6
1	Q	286	SER	3.6
1	P	197	LYS	3.6
1	O	139	HIS	3.5
1	R	83	SER	3.5
1	R	189	VAL	3.5
1	P	177	THR	3.5
1	R	27	ASP	3.5
1	R	201	ALA	3.5
1	Q	197	LYS	3.5
1	O	256	ALA	3.4
1	O	290	VAL	3.4
1	Q	182	SER	3.4
1	P	70	GLY	3.4
1	Q	243	VAL	3.4
1	O	141	TYR	3.4
1	R	68	LEU	3.4
1	Q	71	GLU	3.4
1	P	263	LEU	3.4
1	Q	102	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	Q	269	ALA	3.4
1	Q	92	VAL	3.4
1	R	310	PHE	3.4
1	O	167	ASP	3.3
1	Q	287	GLN	3.3
1	O	184	ALA	3.3
1	O	331	ALA	3.3
1	O	146	LEU	3.3
1	R	248	LEU	3.3
1	O	105	LYS	3.3
1	O	17	LEU	3.3
1	P	64	ASP	3.3
1	P	237	ARG	3.3
1	Q	53	HIS	3.3
1	Q	51	SER	3.3
1	Q	301	LYS	3.3
1	R	211	PRO	3.2
1	O	212	ALA	3.2
1	P	67	LEU	3.2
1	P	141	TYR	3.2
1	R	308	ASP	3.2
1	R	302	ALA	3.2
1	Q	263	LEU	3.2
1	R	225	PRO	3.2
1	O	248	LEU	3.2
1	P	161	LEU	3.2
1	O	246	VAL	3.1
1	P	186	GLN	3.1
1	O	178	THR	3.1
1	P	98	SER	3.1
1	O	71	GLU	3.1
1	P	268	ALA	3.1
1	Q	181	ALA	3.1
1	P	44	CYS	3.1
1	P	222	LYS	3.1
1	Q	268	ALA	3.1
1	O	314	VAL	3.1
1	Q	172	VAL	3.1
1	O	316	TRP	3.1
1	P	271	GLY	3.1
1	P	71	GLU	3.0
1	Q	187	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	334	ILE	3.0
1	R	159	ALA	3.0
1	P	336	THR	3.0
1	P	147	ILE	3.0
1	R	252	LEU	3.0
1	O	136	ILE	3.0
1	P	246	VAL	3.0
1	O	27	ASP	3.0
1	P	317	TYR	3.0
1	Q	257	LYS	3.0
1	O	311	PHE	3.0
1	R	174	GLY	3.0
1	Q	111	HIS	3.0
1	R	67	LEU	3.0
1	Q	256	ALA	3.0
1	Q	167	ASP	3.0
1	R	66	PHE	3.0
1	P	3	ALA	2.9
1	R	316	TRP	2.9
1	Q	336	THR	2.9
1	O	43	LEU	2.9
1	O	84	GLN	2.9
1	O	330	LEU	2.9
1	P	116	ALA	2.9
1	O	171	ILE	2.9
1	R	28	ILE	2.9
1	O	66	PHE	2.9
1	P	169	PHE	2.9
1	Q	246	VAL	2.9
1	R	244	SER	2.9
1	P	269	ALA	2.9
1	O	14	ILE	2.9
1	Q	136	ILE	2.9
1	O	196	GLY	2.9
1	P	302	ALA	2.9
1	O	34	ASN	2.9
1	P	252	LEU	2.9
1	O	201	ALA	2.9
1	Q	223	VAL	2.9
1	O	103	LEU	2.9
1	O	142	ASP	2.9
1	P	286	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	Q	34	ASN	2.8
1	Q	88	GLY	2.8
1	O	175	LEU	2.8
1	P	227	LEU	2.8
1	P	234	VAL	2.8
1	R	246	VAL	2.8
1	R	237	ARG	2.8
1	O	46	LEU	2.8
1	O	321	TRP	2.8
1	P	244	SER	2.8
1	Q	174	GLY	2.8
1	R	132	TYR	2.8
1	R	228	ASN	2.8
1	Q	66	PHE	2.8
1	O	284	VAL	2.8
1	O	53	HIS	2.8
1	O	118	LYS	2.8
1	R	74	VAL	2.8
1	R	92	VAL	2.8
1	O	271	GLY	2.8
1	R	142	ASP	2.8
1	R	297	ILE	2.8
1	Q	220	VAL	2.8
1	R	314	VAL	2.8
1	P	36	PRO	2.8
1	Q	15	GLY	2.8
1	O	64	ASP	2.8
1	R	129	THR	2.8
1	O	317	TYR	2.8
1	Q	284	VAL	2.8
1	R	255	PRO	2.8
1	P	175	LEU	2.8
1	R	128	ASP	2.8
1	O	183	THR	2.8
1	Q	90	CYS	2.8
1	O	77	PHE	2.7
1	P	289	PHE	2.7
1	Q	74	VAL	2.7
1	Q	108	ALA	2.7
1	R	71	GLU	2.8
1	R	263	LEU	2.7
1	Q	104	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	115	GLY	2.7
1	O	177	THR	2.7
1	P	180	HIS	2.7
1	O	190	ASP	2.7
1	R	271	GLY	2.7
1	P	21	ALA	2.7
1	R	182	SER	2.7
1	R	79	GLU	2.7
1	R	164	VAL	2.7
1	P	109	SER	2.7
1	P	217	ALA	2.7
1	R	212	ALA	2.7
1	O	285	VAL	2.7
1	Q	314	VAL	2.7
1	Q	180	HIS	2.7
1	R	139	HIS	2.7
1	R	180	HIS	2.7
1	O	98	SER	2.7
1	P	235	ALA	2.7
1	Q	201	ALA	2.7
1	Q	258	TYR	2.7
1	P	164	VAL	2.7
1	P	284	VAL	2.7
1	R	178	THR	2.7
1	O	303	GLY	2.7
1	O	130	PRO	2.7
1	R	286	SER	2.7
1	P	212	ALA	2.7
1	Q	72	LYS	2.7
1	O	286	SER	2.6
1	P	270	GLU	2.6
1	Q	9	ASN	2.6
1	Q	63	ALA	2.6
1	P	49	TYR	2.6
1	O	107	LEU	2.6
1	R	152	SER	2.6
1	Q	235	ALA	2.6
1	O	88	GLY	2.6
1	R	4	THR	2.6
1	R	169	PHE	2.6
1	P	211	PRO	2.6
1	P	287	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	Q	166	ASN	2.6
1	O	111	HIS	2.6
1	R	235	ALA	2.6
1	R	242	THR	2.6
1	Q	148	VAL	2.6
1	Q	273	LEU	2.6
1	R	203	ARG	2.6
1	P	22	ALA	2.6
1	R	64	ASP	2.6
1	Q	178	THR	2.6
1	O	176	MET	2.6
1	Q	332	VAL	2.6
1	P	221	GLY	2.6
1	Q	3	ALA	2.6
1	R	46	LEU	2.6
1	Q	31	VAL	2.6
1	Q	138	HIS	2.6
1	P	26	LYS	2.6
1	P	122	SER	2.5
1	Q	248	LEU	2.5
1	R	298	PHE	2.5
1	O	319	ASN	2.5
1	R	216	ALA	2.5
1	O	109	SER	2.5
1	R	253	GLN	2.5
1	Q	275	GLY	2.5
1	R	58	CYS	2.5
1	O	49	TYR	2.5
1	O	108	ALA	2.5
1	P	165	ILE	2.5
1	O	267	LYS	2.5
1	Q	302	ALA	2.5
1	Q	297	ILE	2.5
1	Q	200	ARG	2.5
1	O	202	GLY	2.5
1	Q	234	VAL	2.5
1	R	11	PHE	2.5
1	Q	140	GLN	2.5
1	P	193	SER	2.5
1	R	190	ASP	2.5
1	P	104	THR	2.5
1	Q	139	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	213	SER	2.4
1	Q	244	SER	2.4
1	R	51	SER	2.4
1	O	151	ALA	2.4
1	O	289	PHE	2.4
1	Q	23	PHE	2.4
1	O	335	THR	2.4
1	P	256	ALA	2.4
1	Q	310	PHE	2.4
1	R	290	VAL	2.4
1	O	70	GLY	2.4
1	P	51	SER	2.4
1	P	306	LEU	2.4
1	O	3	ALA	2.4
1	P	331	ALA	2.4
1	R	284	VAL	2.4
1	R	321	TRP	2.4
1	R	265	ILE	2.4
1	Q	300	MET	2.4
1	O	51	SER	2.4
1	P	132	TYR	2.4
1	O	309	ASN	2.4
1	R	34	ASN	2.4
1	R	273	LEU	2.4
1	P	10	GLY	2.4
1	P	111	HIS	2.4
1	O	249	VAL	2.4
1	P	157	CYS	2.4
1	P	290	VAL	2.4
1	R	208	ASN	2.4
1	R	334	ILE	2.4
1	Q	38	MET	2.4
1	R	289	PHE	2.4
1	P	144	LYS	2.3
1	P	53	HIS	2.3
1	Q	24	GLY	2.3
1	R	323	TYR	2.3
1	Q	199	TRP	2.3
1	Q	288	ASP	2.3
1	O	69	ILE	2.3
1	O	47	LEU	2.3
1	P	309	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	129	THR	2.3
1	O	110	SER	2.3
1	P	81	ASP	2.3
1	Q	324	SER	2.3
1	Q	169	PHE	2.3
1	P	215	GLY	2.3
1	Q	218	LYS	2.3
1	O	153	CYS	2.3
1	O	227	LEU	2.3
1	P	143	THR	2.3
1	P	223	VAL	2.3
1	P	82	PRO	2.3
1	Q	255	PRO	2.3
1	O	154	THR	2.3
1	Q	49	TYR	2.3
1	O	35	ASP	2.3
1	P	38	MET	2.3
1	R	88	GLY	2.3
1	P	34	ASN	2.3
1	R	257	LYS	2.3
1	R	295	SER	2.3
1	Q	202	GLY	2.2
1	Q	322	GLY	2.2
1	P	153	CYS	2.2
1	R	157	CYS	2.2
1	Q	321	TRP	2.2
1	P	201	ALA	2.2
1	O	4	THR	2.2
1	Q	103	LEU	2.2
1	R	202	GLY	2.2
1	O	199	TRP	2.2
1	O	233	GLY	2.2
1	O	268	ALA	2.2
1	P	123	ALA	2.2
1	P	335	THR	2.2
1	R	303	GLY	2.2
1	R	336	THR	2.2
1	R	6	LEU	2.2
1	R	50	ASP	2.2
1	R	111	HIS	2.2
1	O	106	GLU	2.2
1	O	200	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	203	ARG	2.2
1	Q	319	ASN	2.2
1	Q	325	ASN	2.2
1	P	92	VAL	2.2
1	P	95	VAL	2.2
1	P	314	VAL	2.2
1	Q	164	VAL	2.2
1	R	234	VAL	2.2
1	O	23	PHE	2.2
1	P	310	PHE	2.2
1	Q	37	PHE	2.2
1	Q	114	GLY	2.2
1	P	264	GLU	2.2
1	Q	155	THR	2.2
1	P	324	SER	2.2
1	Q	260	GLU	2.2
1	P	119	VAL	2.2
1	P	261	VAL	2.2
1	Q	65	GLY	2.2
1	Q	271	GLY	2.2
1	P	183	THR	2.2
1	R	143	THR	2.2
1	P	46	LEU	2.2
1	Q	40	LEU	2.2
1	Q	304	LEU	2.2
1	O	144	LYS	2.1
1	O	145	GLN	2.2
1	P	73	LYS	2.1
1	P	118	LYS	2.1
1	P	30	VAL	2.1
1	O	287	GLN	2.1
1	Q	211	PRO	2.1
1	R	125	PRO	2.1
1	O	307	ASN	2.1
1	O	327	VAL	2.1
1	P	56	PHE	2.1
1	Q	84	GLN	2.1
1	R	84	GLN	2.1
1	Q	17	LEU	2.1
1	P	303	GLY	2.1
1	R	191	GLY	2.1
1	O	214	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	99	THR	2.1
1	O	263	LEU	2.1
1	P	250	CYS	2.1
1	R	183	THR	2.1
1	P	203	ARG	2.1
1	P	260	GLU	2.1
1	P	65	GLY	2.1
1	R	54	GLY	2.1
1	R	86	PRO	2.1
1	R	14	ILE	2.1
1	P	304	LEU	2.1
1	Q	64	ASP	2.1
1	Q	299	ASP	2.1
1	P	321	TRP	2.1
1	Q	305	ALA	2.1
1	O	74	VAL	2.1
1	P	110	SER	2.1
1	R	115	GLY	2.1
1	P	125	PRO	2.1
1	P	112	LEU	2.1
1	R	161	LEU	2.1
1	Q	183	THR	2.1
1	R	269	ALA	2.1
1	O	157	CYS	2.1
1	O	170	GLY	2.1
1	Q	10	GLY	2.1
1	Q	222	LYS	2.0
1	O	216	ALA	2.0
1	R	110	SER	2.0
1	O	124	PRO	2.0
1	P	253	GLN	2.0
1	Q	186	GLN	2.0
1	P	142	ASP	2.0
1	Q	81	ASP	2.0
1	R	167	ASP	2.0
1	P	17	LEU	2.0
1	Q	137	ASN	2.0
1	R	319	ASN	2.0
1	O	140	GLN	2.0
1	O	221	GLY	2.0
1	O	13	ARG	2.0
1	O	203	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	93	ASP	2.0
1	O	148	VAL	2.0
1	P	301	LYS	2.0
1	O	132	TYR	2.0
1	R	69	ILE	2.0
1	Q	115	GLY	2.0
1	P	200	ARG	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	NAD	Q	501	44/44	0.81	0.33	1.15	57,67,70,70	0
3	AES	P	602	13/13	0.76	0.25	-0.16	63,65,73,75	0
4	GOL	R	903	6/6	0.66	0.23	-0.27	58,60,61,62	0
2	NAD	P	701	44/44	0.92	0.23	-0.36	38,44,48,49	0
2	NAD	O	801	44/44	0.92	0.21	-0.77	33,44,54,56	0
2	NAD	R	901	44/44	0.94	0.18	-0.97	31,41,48,48	0
4	GOL	R	503	6/6	0.77	0.19	-	76,78,79,82	0
3	AES	O	601	13/13	0.82	0.23	-	67,75,81,82	0
4	GOL	P	703	6/6	0.75	0.36	-	59,64,66,66	0
3	AES	R	603	13/13	0.79	0.24	-	62,67,77,79	0
4	GOL	O	804	6/6	0.79	0.18	-	72,74,76,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.