



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 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 (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

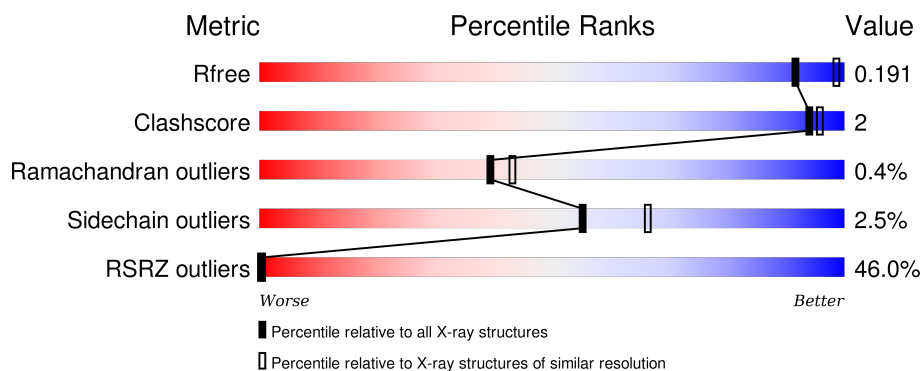
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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>49%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	P	345	<div> <div>45%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	Q	345	<div> <div>46%</div> <div>90%</div> <div>6%</div> <div>..</div> </div>
1	R	345	<div> <div>39%</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:

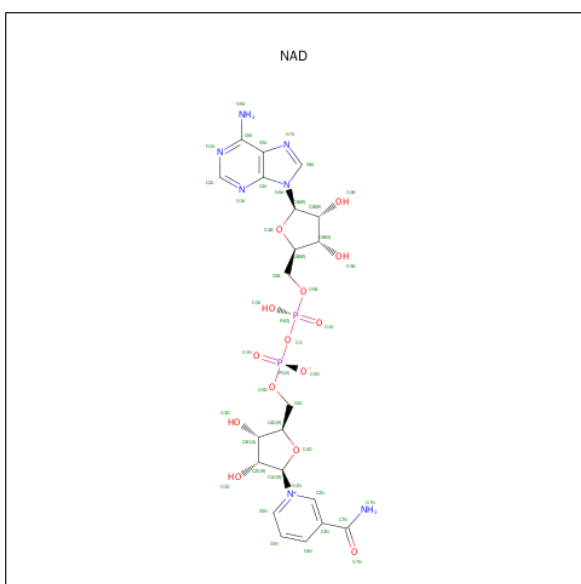
Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
O	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
O	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-1	HIS	-	EXPRESSION TAG	UNP 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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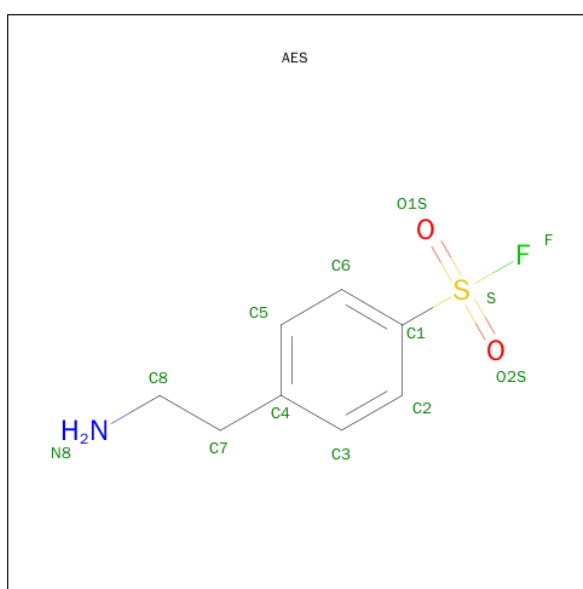
Chain	Residue	Modelled	Actual	Comment	Reference
P	337	SER	ASN	ENGINEERED	UNP Q8T6B1
Q	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-2	HIS	-	EXPRESSION TAG	UNP 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<sub>8</sub>H<sub>10</sub>FN<sub>2</sub>O<sub>2</sub>S).



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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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		

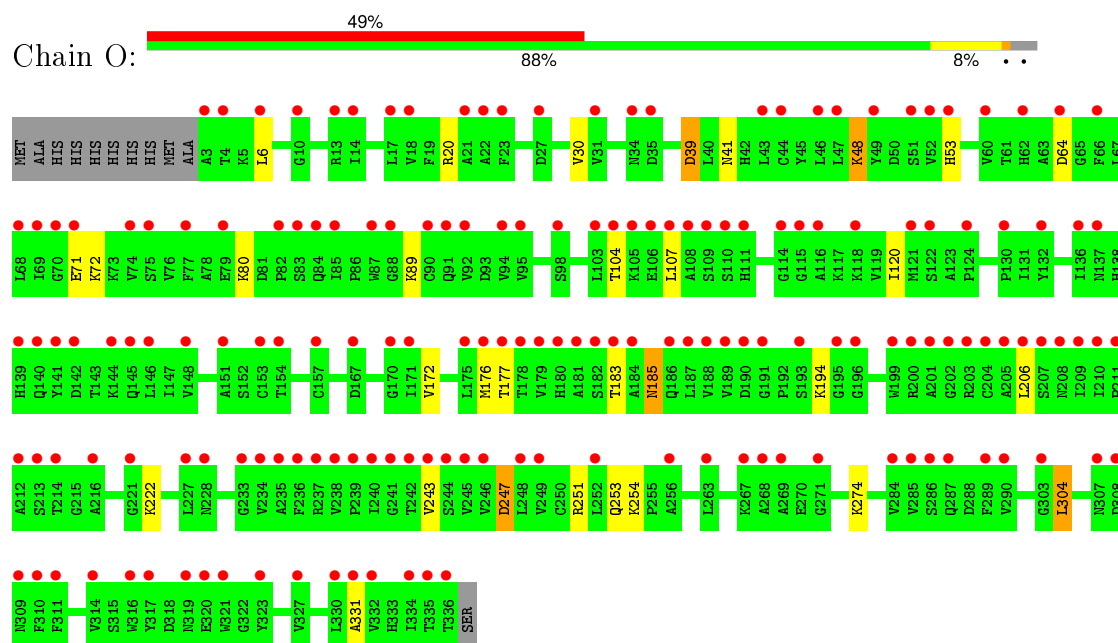
- Molecule 5 is water.

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		

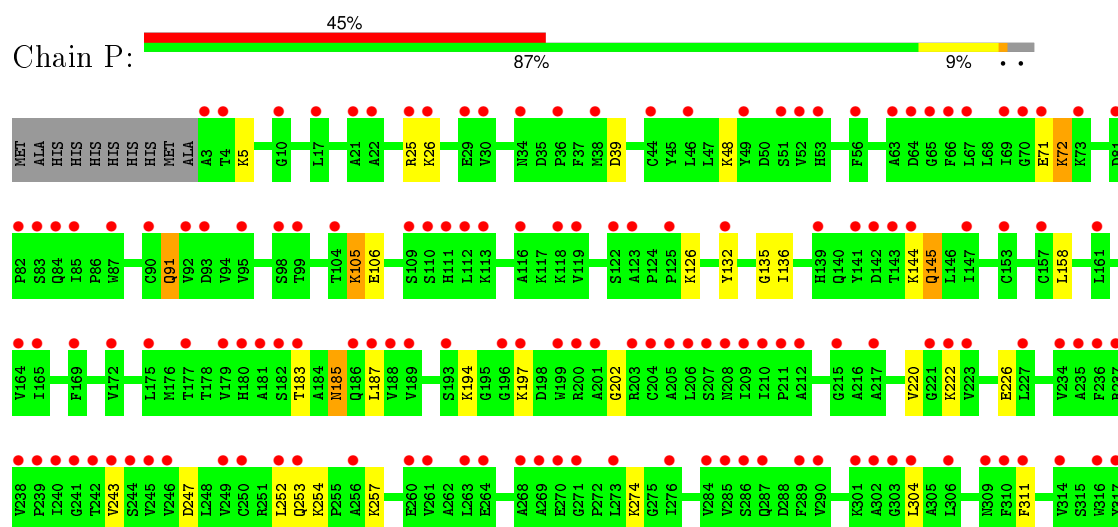
### 3 Residue-property plots

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



- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.33 Å 104.58 Å 90.84 Å 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 2.24 Å)	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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 56935 reflections	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, 0.375 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: 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

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:185:ASN:HD22	1:O:185:ASN:N	2.03	0.56
1:O:104:THR:HG22	1:O:107:LEU:HD12	1.86	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:P:132:TYR:OH	1:P:145:GLN:OE1	2.14	0.46
1:O:206:LEU:HG	1:R:206:LEU:HG	1.96	0.46
1:Q:242:THR:HG23	1:Q:243:VAL:HG23	1.98	0.45
1:Q:12:GLY:HA3	2:Q:501:NAD:O5B	2.16	0.45
1:O:20:ARG:NH2	1:O:53:HIS:O	2.50	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:N	1:R:206:LEU:HD12	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%)	46	52
1	P	332/345 (96%)	314 (95%)	17 (5%)	1 (0%)	46	52
1	Q	332/345 (96%)	313 (94%)	17 (5%)	2 (1%)	30	30
1	R	332/345 (96%)	310 (93%)	21 (6%)	1 (0%)	46	52
All	All	1328/1380 (96%)	1251 (94%)	72 (5%)	5 (0%)	39	43

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%)	55	66
1	P	277/286 (97%)	269 (97%)	8 (3%)	50	60
1	Q	277/286 (97%)	274 (99%)	3 (1%)	80	88
1	R	277/286 (97%)	267 (96%)	10 (4%)	42	51
All	All	1108/1144 (97%)	1080 (98%)	28 (2%)	55	66

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	-	11,13,13	0.53	0	17,18,18	1.86	3 (17%)
2	NAD	O	801	-	38,48,48	1.61	3 (7%)	47,73,73	2.00	5 (10%)
4	GOL	O	804	-	5,5,5	0.32	0	5,5,5	0.21	0
3	AES	P	602	-	11,13,13	0.52	0	17,18,18	1.92	3 (17%)
2	NAD	P	701	-	38,48,48	1.62	3 (7%)	47,73,73	2.04	4 (8%)
4	GOL	P	703	-	5,5,5	0.34	0	5,5,5	0.29	0
2	NAD	Q	501	-	38,48,48	1.71	3 (7%)	47,73,73	2.08	4 (8%)
4	GOL	R	503	-	5,5,5	0.31	0	5,5,5	0.31	0
3	AES	R	603	-	11,13,13	0.52	0	17,18,18	1.90	3 (17%)
2	NAD	R	901	-	38,48,48	1.61	3 (7%)	47,73,73	2.09	4 (8%)
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	2.55	1.38	1.33
2	P	701	NAD	C2A-N1A	2.73	1.39	1.33
2	O	801	NAD	C2A-N1A	2.78	1.39	1.33
2	Q	501	NAD	C2A-N1A	2.80	1.39	1.33
2	P	701	NAD	C2A-N3A	3.61	1.38	1.32
2	Q	501	NAD	C2A-N3A	3.68	1.38	1.32
2	O	801	NAD	C2A-N3A	3.70	1.38	1.32
2	R	901	NAD	C2A-N3A	3.83	1.39	1.32
2	R	901	NAD	O7N-C7N	7.60	1.40	1.24
2	O	801	NAD	O7N-C7N	7.70	1.40	1.24
2	P	701	NAD	O7N-C7N	7.78	1.40	1.24
2	Q	501	NAD	O7N-C7N	8.44	1.42	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	501	NAD	N3A-C2A-N1A	-12.10	119.63	128.89
2	R	901	NAD	N3A-C2A-N1A	-11.92	119.77	128.89
2	O	801	NAD	N3A-C2A-N1A	-11.30	120.24	128.89
2	P	701	NAD	N3A-C2A-N1A	-11.26	120.27	128.89
3	P	602	AES	O2S-S-C1	-6.33	103.88	110.73
3	R	603	AES	O2S-S-C1	-5.49	104.79	110.73
3	O	601	AES	O2S-S-C1	-4.89	105.43	110.73
3	O	601	AES	O1S-S-C1	-4.61	105.75	110.73
3	R	603	AES	O1S-S-C1	-4.04	106.35	110.73
2	Q	501	NAD	PN-O3-PA	-3.47	123.00	132.73
2	R	901	NAD	C4A-C5A-N7A	-2.78	106.92	109.48
2	O	801	NAD	PN-O3-PA	-2.74	125.04	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	602	AES	O1S-S-C1	-2.68	107.83	110.73
2	R	901	NAD	C1B-N9A-C4A	-2.66	122.93	126.94
2	O	801	NAD	C4A-C5A-N7A	-2.54	107.15	109.48
2	P	701	NAD	PN-O3-PA	-2.49	125.75	132.73
2	O	801	NAD	C1B-N9A-C4A	-2.40	123.32	126.94
2	Q	501	NAD	C1B-N9A-C4A	-2.27	123.52	126.94
2	P	701	NAD	C1B-N9A-C4A	-2.16	123.68	126.94
3	P	602	AES	F-S-C1	2.77	108.77	102.39
3	O	601	AES	F-S-C1	2.79	108.82	102.39
3	R	603	AES	F-S-C1	2.97	109.23	102.39
2	Q	501	NAD	O4D-C1D-N1N	3.16	111.60	108.13
2	R	901	NAD	O4D-C1D-N1N	3.23	111.67	108.13
2	O	801	NAD	O4D-C1D-N1N	3.45	111.92	108.13
2	P	701	NAD	O4D-C1D-N1N	5.03	113.66	108.13

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%)	2.34	170 (50%) <b>0</b> <b>0</b>	57, 67, 80, 88	18 (5%)
1	P	334/345 (96%)	2.21	154 (46%) <b>0</b> <b>0</b>	51, 68, 84, 88	21 (6%)
1	Q	334/345 (96%)	2.29	158 (47%) <b>0</b> <b>0</b>	77, 88, 101, 114	17 (5%)
1	R	334/345 (96%)	2.00	133 (39%) <b>0</b> <b>0</b>	49, 61, 75, 89	14 (4%)
All	All	1336/1380 (96%)	2.21	615 (46%) <b>0</b> <b>0</b>	49, 69, 94, 114	70 (5%)

All (615) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	90	CYS	9.6
1	Q	217	ALA	9.4
1	P	206	LEU	8.7
1	O	85	ILE	8.4
1	R	206	LEU	8.0
1	P	209	ILE	7.6
1	Q	224	LEU	7.5
1	P	63	ALA	7.5
1	Q	206	LEU	7.3
1	O	240	ILE	7.2
1	Q	221	GLY	7.1
1	Q	209	ILE	6.9
1	O	209	ILE	6.8
1	O	206	LEU	6.8
1	Q	238	VAL	6.8
1	O	238	VAL	6.4
1	O	239	PRO	6.4
1	Q	99	THR	6.3
1	O	92	VAL	6.3
1	Q	240	ILE	6.2
1	P	236	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
1	R	87	TRP	6.2
1	R	114	GLY	6.2
1	O	205	ALA	6.1
1	O	210	ILE	6.0
1	O	82	PRO	6.0
1	R	238	VAL	6.0
1	P	69	ILE	6.0
1	P	240	ILE	6.0
1	P	66	PHE	5.9
1	Q	236	PHE	5.9
1	P	84	GLN	5.9
1	Q	116	ALA	5.9
1	R	52	VAL	5.8
1	R	188	VAL	5.8
1	O	336	THR	5.7
1	P	239	PRO	5.7
1	O	179	VAL	5.7
1	P	179	VAL	5.7
1	R	205	ALA	5.7
1	Q	205	ALA	5.6
1	Q	179	VAL	5.6
1	O	188	VAL	5.6
1	R	309	ASN	5.5
1	O	83	SER	5.5
1	R	209	ILE	5.5
1	R	204	CYS	5.4
1	O	241	GLY	5.4
1	P	241	GLY	5.4
1	R	207	SER	5.4
1	P	85	ILE	5.4
1	R	187	LEU	5.3
1	P	205	ALA	5.3
1	P	238	VAL	5.3
1	R	240	ILE	5.3
1	P	207	SER	5.2
1	P	188	VAL	5.2
1	P	189	VAL	5.2
1	Q	109	SER	5.2
1	P	90	CYS	5.2
1	P	83	SER	5.2
1	O	204	CYS	5.2
1	R	239	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	O	87	TRP	5.2
1	Q	239	PRO	5.1
1	P	52	VAL	5.1
1	O	6	LEU	5.0
1	O	236	PHE	5.0
1	O	75	SER	5.0
1	Q	285	VAL	5.0
1	R	179	VAL	5.0
1	O	114	GLY	5.0
1	R	90	CYS	5.0
1	O	235	ALA	5.0
1	O	207	SER	4.9
1	P	87	TRP	4.9
1	Q	207	SER	4.9
1	Q	227	LEU	4.9
1	Q	83	SER	4.9
1	O	187	LEU	4.9
1	R	184	ALA	4.8
1	O	116	ALA	4.8
1	O	245	VAL	4.8
1	P	196	GLY	4.8
1	R	65	GLY	4.8
1	Q	188	VAL	4.8
1	P	245	VAL	4.7
1	Q	143	THR	4.7
1	O	189	VAL	4.7
1	P	316	TRP	4.7
1	Q	204	CYS	4.6
1	O	104	THR	4.6
1	P	285	VAL	4.6
1	O	68	LEU	4.6
1	O	52	VAL	4.6
1	P	210	ILE	4.6
1	O	94	VAL	4.6
1	Q	317	TYR	4.6
1	P	187	LEU	4.6
1	O	91	GLN	4.5
1	P	204	CYS	4.5
1	Q	165	ILE	4.5
1	Q	242	THR	4.5
1	R	241	GLY	4.5
1	Q	52	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	O	234	VAL	4.5
1	Q	210	ILE	4.5
1	O	22	ALA	4.5
1	Q	316	TRP	4.4
1	P	139	HIS	4.4
1	R	243	VAL	4.4
1	O	182	SER	4.4
1	O	243	VAL	4.4
1	Q	245	VAL	4.4
1	O	334	ILE	4.4
1	R	311	PHE	4.4
1	O	252	LEU	4.4
1	Q	290	VAL	4.4
1	Q	241	GLY	4.3
1	R	332	VAL	4.3
1	R	210	ILE	4.3
1	P	172	VAL	4.3
1	P	332	VAL	4.3
1	Q	309	ASN	4.3
1	O	10	GLY	4.2
1	P	181	ALA	4.2
1	Q	253	GLN	4.2
1	O	269	ALA	4.2
1	Q	308	ASP	4.2
1	O	242	THR	4.2
1	R	236	PHE	4.2
1	R	245	VAL	4.2
1	P	242	THR	4.1
1	R	181	ALA	4.1
1	Q	170	GLY	4.1
1	Q	228	ASN	4.1
1	O	180	HIS	4.1
1	Q	142	ASP	4.0
1	Q	141	TYR	4.0
1	Q	168	ARG	4.0
1	P	182	SER	4.0
1	Q	237	ARG	3.9
1	Q	311	PHE	3.9
1	P	208	ASN	3.9
1	Q	252	LEU	3.9
1	R	285	VAL	3.9
1	Q	208	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	O	79	GLU	3.9
1	Q	132	TYR	3.9
1	Q	189	VAL	3.9
1	R	186	GLN	3.9
1	P	243	VAL	3.9
1	Q	128	ASP	3.9
1	P	311	PHE	3.8
1	O	308	ASP	3.8
1	O	237	ARG	3.8
1	O	332	VAL	3.8
1	P	273	LEU	3.8
1	Q	328	LEU	3.8
1	O	181	ALA	3.7
1	R	112	LEU	3.7
1	O	208	ASN	3.7
1	O	228	ASN	3.7
1	O	211	PRO	3.7
1	Q	87	TRP	3.7
1	O	186	GLN	3.7
1	O	244	SER	3.7
1	Q	286	SER	3.7
1	R	317	TYR	3.7
1	P	25	ARG	3.7
1	P	113	LYS	3.7
1	O	139	HIS	3.7
1	R	83	SER	3.7
1	R	189	VAL	3.7
1	P	197	LYS	3.6
1	P	177	THR	3.6
1	O	290	VAL	3.6
1	R	201	ALA	3.6
1	R	27	ASP	3.6
1	Q	243	VAL	3.6
1	O	256	ALA	3.6
1	Q	182	SER	3.6
1	P	70	GLY	3.6
1	R	68	LEU	3.6
1	Q	197	LYS	3.5
1	Q	92	VAL	3.5
1	Q	269	ALA	3.5
1	P	263	LEU	3.5
1	O	141	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	Q	102	PHE	3.5
1	Q	71	GLU	3.5
1	R	310	PHE	3.5
1	O	331	ALA	3.5
1	O	167	ASP	3.5
1	O	184	ALA	3.5
1	O	146	LEU	3.5
1	R	248	LEU	3.5
1	Q	287	GLN	3.4
1	O	17	LEU	3.4
1	Q	53	HIS	3.4
1	P	64	ASP	3.4
1	O	105	LYS	3.4
1	Q	51	SER	3.4
1	R	211	PRO	3.4
1	O	212	ALA	3.4
1	P	67	LEU	3.4
1	P	237	ARG	3.4
1	Q	301	LYS	3.3
1	R	308	ASP	3.3
1	R	302	ALA	3.3
1	P	141	TYR	3.3
1	Q	263	LEU	3.3
1	R	225	PRO	3.3
1	O	246	VAL	3.3
1	O	248	LEU	3.3
1	P	161	LEU	3.3
1	O	178	THR	3.3
1	P	44	CYS	3.3
1	P	268	ALA	3.3
1	Q	181	ALA	3.3
1	P	98	SER	3.2
1	O	314	VAL	3.2
1	Q	172	VAL	3.2
1	P	186	GLN	3.2
1	Q	268	ALA	3.2
1	O	71	GLU	3.2
1	O	316	TRP	3.2
1	P	271	GLY	3.2
1	P	334	ILE	3.2
1	Q	187	LEU	3.2
1	R	159	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	P	336	THR	3.2
1	P	147	ILE	3.2
1	P	246	VAL	3.2
1	P	222	LYS	3.2
1	O	136	ILE	3.1
1	P	71	GLU	3.1
1	R	252	LEU	3.1
1	O	27	ASP	3.1
1	O	311	PHE	3.1
1	R	174	GLY	3.1
1	Q	256	ALA	3.1
1	Q	111	HIS	3.1
1	R	67	LEU	3.1
1	P	317	TYR	3.1
1	R	66	PHE	3.1
1	O	171	ILE	3.1
1	P	3	ALA	3.1
1	Q	167	ASP	3.1
1	Q	246	VAL	3.1
1	Q	336	THR	3.1
1	R	316	TRP	3.1
1	O	14	ILE	3.1
1	R	28	ILE	3.1
1	P	116	ALA	3.1
1	O	43	LEU	3.1
1	O	330	LEU	3.1
1	Q	257	LYS	3.1
1	O	66	PHE	3.1
1	P	169	PHE	3.1
1	P	269	ALA	3.0
1	Q	136	ILE	3.0
1	R	244	SER	3.0
1	P	302	ALA	3.0
1	O	196	GLY	3.0
1	Q	223	VAL	3.0
1	O	84	GLN	3.0
1	O	34	ASN	3.0
1	O	201	ALA	3.0
1	P	252	LEU	3.0
1	O	103	LEU	3.0
1	P	234	VAL	3.0
1	R	246	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	Q	88	GLY	3.0
1	O	142	ASP	3.0
1	O	175	LEU	3.0
1	P	227	LEU	3.0
1	P	286	SER	3.0
1	O	284	VAL	3.0
1	R	74	VAL	3.0
1	R	92	VAL	3.0
1	O	46	LEU	3.0
1	Q	34	ASN	2.9
1	O	321	TRP	2.9
1	Q	174	GLY	2.9
1	Q	220	VAL	2.9
1	R	314	VAL	2.9
1	P	244	SER	2.9
1	Q	66	PHE	2.9
1	R	297	ILE	2.9
1	O	53	HIS	2.9
1	R	228	ASN	2.9
1	O	271	GLY	2.9
1	Q	90	CYS	2.9
1	Q	284	VAL	2.9
1	R	132	TYR	2.9
1	P	36	PRO	2.9
1	R	129	THR	2.9
1	R	142	ASP	2.9
1	Q	15	GLY	2.9
1	R	237	ARG	2.9
1	Q	74	VAL	2.9
1	O	64	ASP	2.9
1	O	183	THR	2.9
1	R	255	PRO	2.9
1	P	175	LEU	2.9
1	Q	108	ALA	2.9
1	R	128	ASP	2.9
1	O	118	LYS	2.9
1	O	77	PHE	2.9
1	O	317	TYR	2.9
1	P	289	PHE	2.9
1	Q	104	THR	2.9
1	R	263	LEU	2.9
1	R	164	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	115	GLY	2.9
1	O	177	THR	2.9
1	P	21	ALA	2.8
1	P	180	HIS	2.8
1	O	285	VAL	2.8
1	Q	314	VAL	2.8
1	R	71	GLU	2.8
1	R	271	GLY	2.8
1	O	190	ASP	2.8
1	R	182	SER	2.8
1	R	139	HIS	2.8
1	P	217	ALA	2.8
1	R	212	ALA	2.8
1	P	164	VAL	2.8
1	P	284	VAL	2.8
1	P	109	SER	2.8
1	Q	180	HIS	2.8
1	R	180	HIS	2.8
1	P	235	ALA	2.8
1	Q	201	ALA	2.8
1	R	178	THR	2.8
1	R	79	GLU	2.8
1	O	98	SER	2.8
1	Q	258	TYR	2.8
1	O	303	GLY	2.8
1	P	212	ALA	2.8
1	O	130	PRO	2.8
1	R	286	SER	2.8
1	Q	63	ALA	2.8
1	O	286	SER	2.8
1	Q	148	VAL	2.8
1	O	107	LEU	2.8
1	Q	9	ASN	2.8
1	Q	235	ALA	2.8
1	R	4	THR	2.8
1	P	270	GLU	2.8
1	R	152	SER	2.7
1	O	88	GLY	2.7
1	R	169	PHE	2.7
1	P	49	TYR	2.7
1	P	211	PRO	2.7
1	R	235	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	R	242	THR	2.7
1	Q	72	LYS	2.7
1	O	111	HIS	2.7
1	Q	166	ASN	2.7
1	Q	332	VAL	2.7
1	Q	273	LEU	2.7
1	P	22	ALA	2.7
1	Q	178	THR	2.7
1	Q	31	VAL	2.7
1	P	287	GLN	2.7
1	Q	3	ALA	2.7
1	R	64	ASP	2.7
1	P	221	GLY	2.7
1	O	176	MET	2.7
1	R	46	LEU	2.7
1	R	58	CYS	2.7
1	Q	138	HIS	2.7
1	R	203	ARG	2.7
1	Q	248	LEU	2.7
1	P	122	SER	2.7
1	R	216	ALA	2.7
1	R	298	PHE	2.7
1	O	319	ASN	2.6
1	O	108	ALA	2.6
1	O	109	SER	2.6
1	P	165	ILE	2.6
1	Q	275	GLY	2.6
1	Q	234	VAL	2.6
1	Q	297	ILE	2.6
1	Q	302	ALA	2.6
1	P	26	LYS	2.6
1	O	49	TYR	2.6
1	R	253	GLN	2.6
1	O	202	GLY	2.6
1	R	11	PHE	2.6
1	P	104	THR	2.6
1	O	267	LYS	2.6
1	P	193	SER	2.6
1	Q	139	HIS	2.6
1	R	190	ASP	2.6
1	O	151	ALA	2.6
1	Q	140	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	290	VAL	2.6
1	O	335	THR	2.6
1	Q	200	ARG	2.6
1	O	289	PHE	2.6
1	Q	23	PHE	2.6
1	O	213	SER	2.6
1	Q	244	SER	2.6
1	R	51	SER	2.6
1	P	256	ALA	2.6
1	P	331	ALA	2.6
1	R	284	VAL	2.6
1	Q	310	PHE	2.5
1	O	70	GLY	2.5
1	O	3	ALA	2.5
1	P	306	LEU	2.5
1	R	265	ILE	2.5
1	P	157	CYS	2.5
1	P	51	SER	2.5
1	R	321	TRP	2.5
1	O	249	VAL	2.5
1	P	290	VAL	2.5
1	Q	300	MET	2.5
1	R	273	LEU	2.5
1	O	51	SER	2.5
1	P	10	GLY	2.5
1	P	111	HIS	2.5
1	R	334	ILE	2.5
1	O	309	ASN	2.5
1	R	34	ASN	2.5
1	P	132	TYR	2.5
1	R	208	ASN	2.5
1	R	289	PHE	2.5
1	O	153	CYS	2.5
1	Q	24	GLY	2.5
1	P	53	HIS	2.5
1	Q	38	MET	2.5
1	Q	199	TRP	2.5
1	O	69	ILE	2.5
1	Q	129	THR	2.4
1	O	47	LEU	2.4
1	Q	288	ASP	2.4
1	R	323	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	223	VAL	2.4
1	P	144	LYS	2.4
1	Q	169	PHE	2.4
1	P	215	GLY	2.4
1	O	110	SER	2.4
1	P	143	THR	2.4
1	P	309	ASN	2.4
1	Q	324	SER	2.4
1	P	81	ASP	2.4
1	O	227	LEU	2.4
1	O	154	THR	2.4
1	P	82	PRO	2.4
1	Q	255	PRO	2.4
1	P	153	CYS	2.4
1	R	157	CYS	2.4
1	Q	49	TYR	2.4
1	O	35	ASP	2.4
1	Q	218	LYS	2.4
1	R	88	GLY	2.4
1	P	38	MET	2.4
1	Q	202	GLY	2.4
1	Q	322	GLY	2.4
1	R	295	SER	2.4
1	Q	321	TRP	2.4
1	O	4	THR	2.4
1	P	123	ALA	2.4
1	P	201	ALA	2.4
1	P	34	ASN	2.3
1	Q	103	LEU	2.3
1	R	202	GLY	2.3
1	Q	164	VAL	2.3
1	R	234	VAL	2.3
1	O	268	ALA	2.3
1	P	335	THR	2.3
1	R	336	THR	2.3
1	O	199	TRP	2.3
1	O	233	GLY	2.3
1	R	303	GLY	2.3
1	R	6	LEU	2.3
1	R	111	HIS	2.3
1	R	257	LYS	2.3
1	P	92	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	95	VAL	2.3
1	P	314	VAL	2.3
1	R	50	ASP	2.3
1	P	119	VAL	2.3
1	P	261	VAL	2.3
1	Q	155	THR	2.3
1	Q	319	ASN	2.3
1	Q	325	ASN	2.3
1	O	23	PHE	2.3
1	P	310	PHE	2.3
1	Q	37	PHE	2.3
1	Q	114	GLY	2.3
1	O	106	GLU	2.3
1	P	30	VAL	2.3
1	P	183	THR	2.3
1	R	143	THR	2.3
1	O	200	ARG	2.3
1	Q	65	GLY	2.3
1	Q	203	ARG	2.3
1	Q	271	GLY	2.3
1	P	324	SER	2.3
1	P	46	LEU	2.3
1	Q	40	LEU	2.3
1	Q	304	LEU	2.3
1	P	264	GLU	2.3
1	Q	260	GLU	2.3
1	O	327	VAL	2.3
1	Q	211	PRO	2.2
1	R	125	PRO	2.2
1	P	250	CYS	2.2
1	P	56	PHE	2.2
1	O	307	ASN	2.2
1	O	145	GLN	2.2
1	Q	17	LEU	2.2
1	O	144	LYS	2.2
1	P	303	GLY	2.2
1	R	191	GLY	2.2
1	O	214	THR	2.2
1	P	99	THR	2.2
1	O	287	GLN	2.2
1	P	73	LYS	2.2
1	P	118	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	263	LEU	2.2
1	R	183	THR	2.2
1	R	14	ILE	2.2
1	O	74	VAL	2.2
1	Q	84	GLN	2.2
1	R	84	GLN	2.2
1	O	157	CYS	2.2
1	P	65	GLY	2.2
1	R	54	GLY	2.2
1	P	304	LEU	2.2
1	R	86	PRO	2.2
1	Q	305	ALA	2.2
1	P	321	TRP	2.2
1	Q	64	ASP	2.2
1	Q	299	ASP	2.2
1	R	115	GLY	2.2
1	P	125	PRO	2.2
1	P	112	LEU	2.2
1	R	161	LEU	2.2
1	P	110	SER	2.2
1	Q	183	THR	2.2
1	P	260	GLU	2.2
1	R	269	ALA	2.2
1	O	170	GLY	2.2
1	P	203	ARG	2.2
1	Q	10	GLY	2.2
1	O	216	ALA	2.2
1	O	148	VAL	2.1
1	O	124	PRO	2.1
1	P	17	LEU	2.1
1	R	110	SER	2.1
1	P	142	ASP	2.1
1	Q	81	ASP	2.1
1	R	167	ASP	2.1
1	O	221	GLY	2.1
1	R	69	ILE	2.1
1	Q	137	ASN	2.1
1	R	319	ASN	2.1
1	P	93	ASP	2.1
1	P	253	GLN	2.1
1	Q	186	GLN	2.1
1	Q	115	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	Q	157	CYS	2.1
1	Q	222	LYS	2.1
1	O	62	HIS	2.1
1	O	132	TYR	2.1
1	O	140	GLN	2.1
1	P	4	THR	2.1
1	P	328	LEU	2.1
1	O	191	GLY	2.1
1	O	13	ARG	2.1
1	O	18	VAL	2.1
1	O	193	SER	2.1
1	O	203	ARG	2.1
1	Q	198	ASP	2.1
1	O	310	PHE	2.1
1	P	199	TRP	2.1
1	R	47	LEU	2.1
1	P	301	LYS	2.1
1	Q	54	GLY	2.1
1	O	137	ASN	2.1
1	R	166	ASN	2.1
1	P	200	ARG	2.1
1	P	276	ILE	2.1
1	R	82	PRO	2.1
1	R	247	ASP	2.1
1	O	60	VAL	2.1
1	O	95	VAL	2.1
1	R	153	CYS	2.1
1	O	323	TYR	2.1
1	P	29	GLU	2.1
1	Q	226	GLU	2.1
1	O	21	ALA	2.1
1	O	31	VAL	2.1
1	P	249	VAL	2.1
1	O	195	GLY	2.0
1	O	121	MET	2.0
1	Q	196	GLY	2.0
1	Q	251	ARG	2.0
1	R	9	ASN	2.0
1	R	200	ARG	2.0
1	R	172	VAL	2.0
1	R	177	THR	2.0
1	O	44	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	R	81	ASP	2.0
1	O	320	GLU	2.0
1	Q	277	LEU	2.0
1	O	122	SER	2.0
1	P	323	TYR	2.0
1	Q	58	CYS	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.