



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 04:57 pm GMT

PDB ID : 2B4T  
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 : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

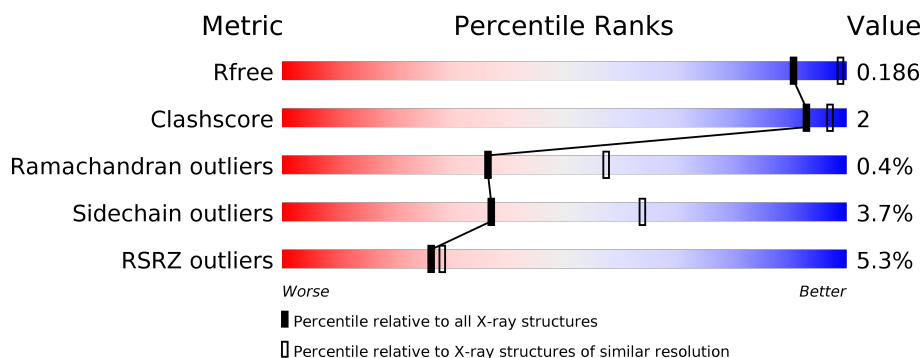
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	345	<div> <div>7%</div> <div>87%</div> <div>8%</div> <div>...</div> </div>
1	P	345	<div> <div>4%</div> <div>86%</div> <div>8%</div> <div>...</div> </div>
1	Q	345	<div> <div>4%</div> <div>87%</div> <div>7%</div> <div>...</div> </div>
1	R	345	<div> <div>6%</div> <div>87%</div> <div>7%</div> <div>...</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10631 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	333	Total	C	N	O	S	56	0	0
			2546	1624	437	472	13			
1	P	333	Total	C	N	O	S	73	0	0
			2546	1624	437	472	13			
1	Q	333	Total	C	N	O	S	57	0	0
			2546	1624	437	472	13			
1	R	333	Total	C	N	O	S	46	0	0
			2546	1624	437	472	13			

There are 44 discrepancies between the modelled and reference sequences:

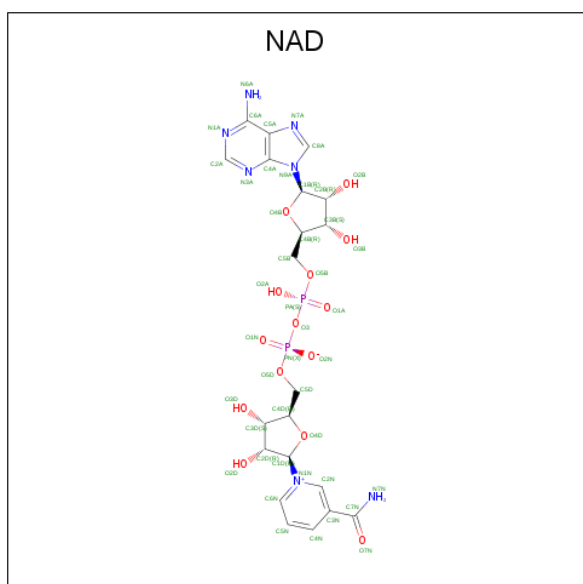
Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
O	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
O	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-1	HIS	-	EXPRESSION TAG	UNP 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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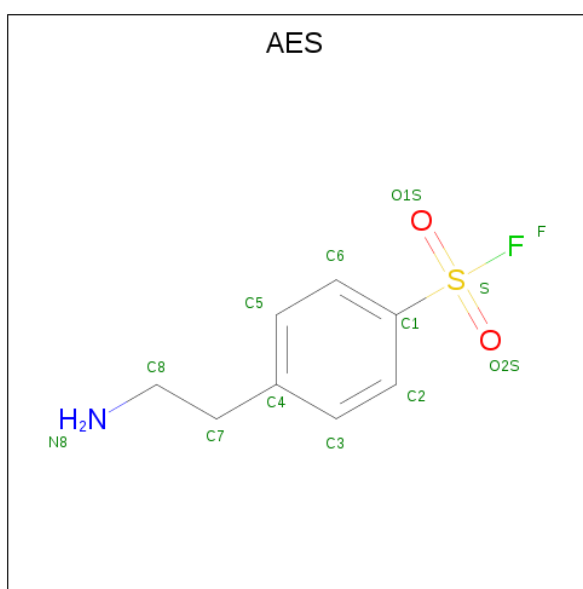
Chain	Residue	Modelled	Actual	Comment	Reference
P	337	SER	ASN	ENGINEERED	UNP Q8T6B1
Q	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-2	HIS	-	EXPRESSION TAG	UNP 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	O	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	Q	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>FNO<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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	65	Total 65 O 65	0	0
4	P	63	Total 63 O 63	0	0

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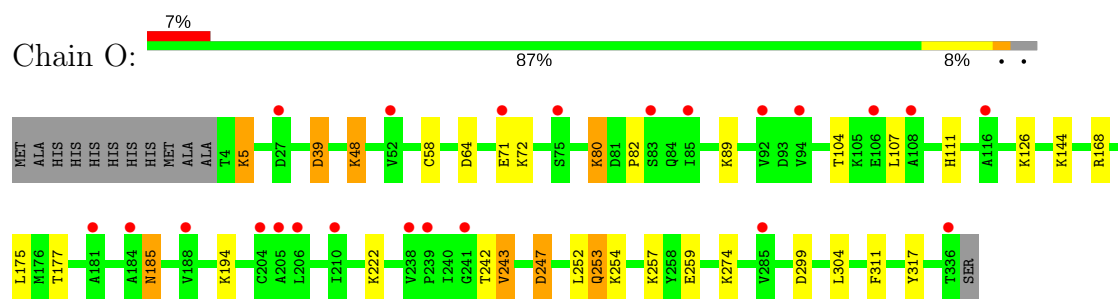
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	49	Total 49	O 49	0	0
4	R	55	Total 55	O 55	0	0

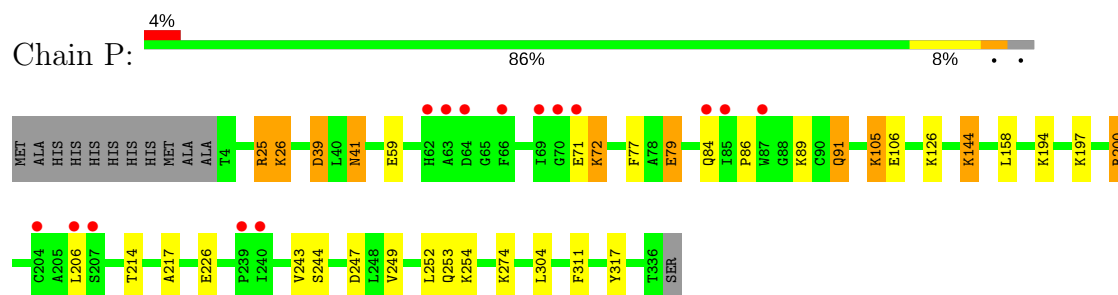
### 3 Residue-property plots [i](#)

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.

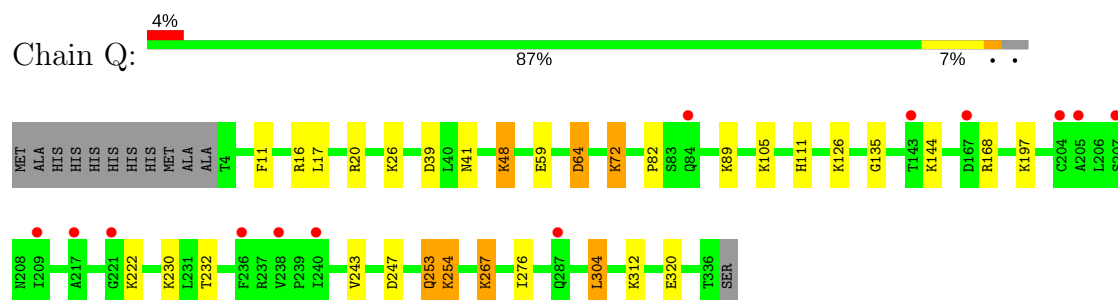
- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase



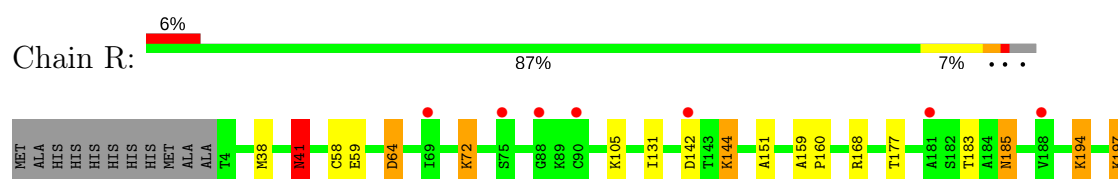
- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

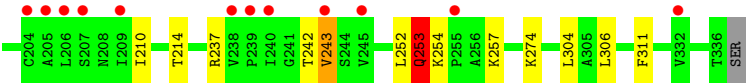


- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase



- 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, $\alpha$ , $\beta$ , $\gamma$	69.69Å 106.06Å 91.06Å 90.00° 107.24° 90.00°	Depositor
Resolution (Å)	43.48 – 2.50 43.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (43.48-2.50) 97.7 (43.48-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.174 , 0.217 0.186 , 0.186	Depositor DCC
$R_{free}$ test set	2115 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: 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	1.44	17/2598 (0.7%)	1.41	22/3521 (0.6%)
1	P	1.68	16/2598 (0.6%)	1.11	30/3521 (0.9%)
1	Q	1.47	14/2598 (0.5%)	1.05	23/3521 (0.7%)
1	R	2.04	13/2598 (0.5%)	1.07	20/3521 (0.6%)
All	All	1.67	60/10392 (0.6%)	1.17	95/14084 (0.7%)

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	P	0	1
1	Q	0	1
1	R	0	2
All	All	0	4

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	253	GLN	CG-CD	78.85	3.32	1.51
1	P	59	GLU	CB-CG	-47.15	0.62	1.52
1	Q	254	LYS	CB-CG	-41.12	0.41	1.52
1	P	25	ARG	CG-CD	-39.20	0.54	1.51
1	Q	230	LYS	CD-CE	-36.30	0.60	1.51

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	39	ASP	CB-CG-OD1	-28.34	92.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	39	ASP	CB-CG-OD2	27.38	142.94	118.30
1	O	71	GLU	CB-CA-C	-26.76	56.89	110.40
1	O	71	GLU	CA-CB-CG	-25.63	57.01	113.40
1	O	64	ASP	CB-CA-C	-24.03	62.34	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	41	ASN	Sidechain
1	Q	253	GLN	Sidechain
1	R	253	GLN	Sidechain
1	R	41	ASN	Sidechain

## 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	2546	0	2573	9	1
1	P	2546	0	2573	10	1
1	Q	2546	0	2573	9	0
1	R	2546	0	2573	10	1
2	O	44	0	26	0	0
2	P	44	0	26	0	0
2	Q	44	0	26	0	0
2	R	44	0	26	0	0
3	O	13	0	10	0	0
3	P	13	0	10	0	0
3	R	13	0	10	0	0
4	O	65	0	0	1	1
4	P	63	0	0	0	0
4	Q	49	0	0	2	0
4	R	55	0	0	1	0
All	All	10631	0	10426	33	2

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.

The worst 5 of 33 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:177:THR:OG1	1:P:247:ASP:OD2	2.08	0.71
1:Q:312:LYS:NZ	1:R:177:THR:OG1	2.27	0.67
1:R:185:ASN:H	1:R:185:ASN:HD22	1.49	0.58
1:P:206:LEU:HD22	4:Q:842:HOH:O	2.04	0.58
1:R:183:THR:OG1	1:R:185:ASN:ND2	2.37	0.57

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:144:LYS:CE	4:O:662:HOH:O[2_545]	1.52	0.68
1:O:253:GLN:NE2	1:R:253:GLN:CG[1_554]	1.95	0.25

## 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	331/345 (96%)	313 (95%)	17 (5%)	1 (0%)	43	64
1	P	331/345 (96%)	311 (94%)	19 (6%)	1 (0%)	43	64
1	Q	331/345 (96%)	310 (94%)	20 (6%)	1 (0%)	43	64
1	R	331/345 (96%)	311 (94%)	18 (5%)	2 (1%)	27	46
All	All	1324/1380 (96%)	1245 (94%)	74 (6%)	5 (0%)	36	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	243	VAL
1	R	243	VAL

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Mol	Chain	Res	Type
1	Q	243	VAL
1	O	243	VAL
1	R	38	MET

### 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%)	267 (96%)	10 (4%)	38	65
1	P	277/286 (97%)	267 (96%)	10 (4%)	38	65
1	Q	277/286 (97%)	267 (96%)	10 (4%)	38	65
1	R	277/286 (97%)	266 (96%)	11 (4%)	34	60
All	All	1108/1144 (97%)	1067 (96%)	41 (4%)	37	64

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	214	THR
1	Q	64	ASP
1	R	194	LYS
1	P	304	LEU
1	Q	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	145	GLN
1	O	185	ASN
1	P	138	HIS
1	Q	140	GLN
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 ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	O	501	-	40,48,48	1.66	3 (7%)	44,73,73	1.78	3 (6%)
3	AES	O	601	-	11,13,13	0.50	0	16,18,18	1.76	2 (12%)
3	AES	P	602	-	11,13,13	0.53	0	16,18,18	1.60	2 (12%)
2	NAD	P	701	-	40,48,48	1.60	3 (7%)	44,73,73	1.73	4 (9%)
2	NAD	Q	801	-	40,48,48	1.77	3 (7%)	44,73,73	1.77	2 (4%)
3	AES	R	603	-	11,13,13	0.57	0	16,18,18	1.83	2 (12%)
2	NAD	R	901	-	40,48,48	1.66	3 (7%)	44,73,73	1.81	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	O	501	-	-	0/22/62/62	0/5/5/5
3	AES	O	601	-	-	0/9/9/9	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AES	P	602	-	-	0/9/9/9	0/1/1/1
2	NAD	P	701	-	-	0/22/62/62	0/5/5/5
2	NAD	Q	801	-	-	0/22/62/62	0/5/5/5
3	AES	R	603	-	-	0/9/9/9	0/1/1/1
2	NAD	R	901	-	-	0/22/62/62	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	701	NAD	C2A-N1A	2.59	1.38	1.33
2	O	501	NAD	C2A-N1A	2.59	1.38	1.33
2	R	901	NAD	C2A-N1A	2.74	1.39	1.33
2	Q	801	NAD	C2A-N1A	3.10	1.39	1.33
2	P	701	NAD	C2A-N3A	4.01	1.38	1.32

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	901	NAD	N3A-C2A-N1A	-10.42	119.94	128.86
2	Q	801	NAD	N3A-C2A-N1A	-10.09	120.23	128.86
2	O	501	NAD	N3A-C2A-N1A	-9.75	120.52	128.86
2	P	701	NAD	N3A-C2A-N1A	-9.49	120.74	128.86
3	R	603	AES	O2S-S-C1	-5.74	104.88	110.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	333/345 (96%)	0.38	23 (6%)	17 17	44, 53, 59, 63	17 (5%)
1	P	333/345 (96%)	0.30	15 (4%)	33 36	44, 52, 63, 68	21 (6%)
1	Q	333/345 (96%)	0.46	13 (3%)	39 42	44, 53, 63, 67	17 (5%)
1	R	333/345 (96%)	0.36	19 (5%)	24 25	46, 52, 59, 67	14 (4%)
All	All	1332/1380 (96%)	0.38	70 (5%)	26 28	44, 53, 61, 68	69 (5%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	63	ALA	5.5
1	P	71	GLU	4.7
1	P	66	PHE	4.3
1	Q	217	ALA	4.1
1	O	85	ILE	3.7

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AES	O	601	13/13	0.85	0.23	56,73,83,85	0
3	AES	P	602	13/13	0.89	0.17	66,68,75,76	0
3	AES	R	603	13/13	0.89	0.18	60,68,76,79	0
2	NAD	Q	801	44/44	0.94	0.20	55,66,74,75	0
2	NAD	O	501	44/44	0.95	0.12	41,52,62,64	0
2	NAD	R	901	44/44	0.96	0.13	44,50,54,54	0
2	NAD	P	701	44/44	0.97	0.12	42,50,53,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.