



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:11 AM GMT

PDB ID : 2B4T
Title : Crystal structure of glyceraldehyde-3-phosphatedehydrogenase 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 full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

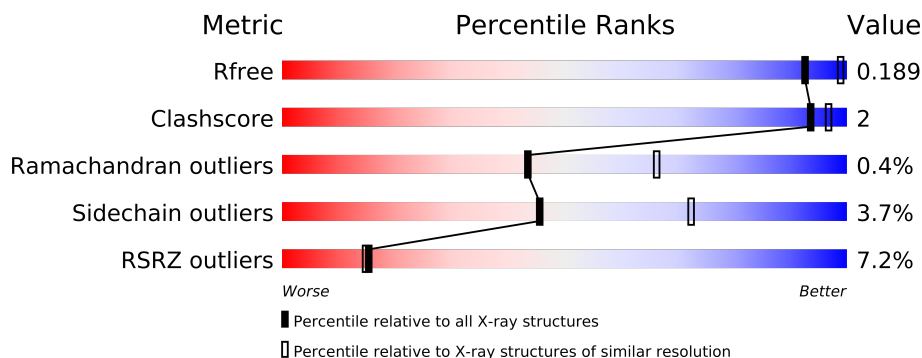
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	O	345	
1	P	345	
1	Q	345	
1	R	345	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10631 atoms, of which 0 are hydrogen and 0 are deuterium.

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-phosphatedehydrogenase.

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:

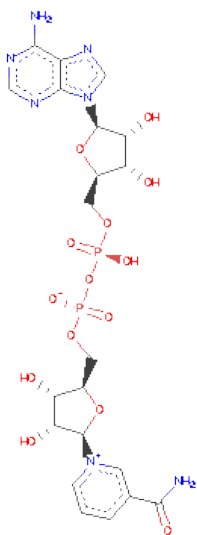
Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
O	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
O	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-2	HIS	-	EXPRESSION TAG	UNP Q8T6B1
O	-1	HIS	-	EXPRESSION TAG	UNP 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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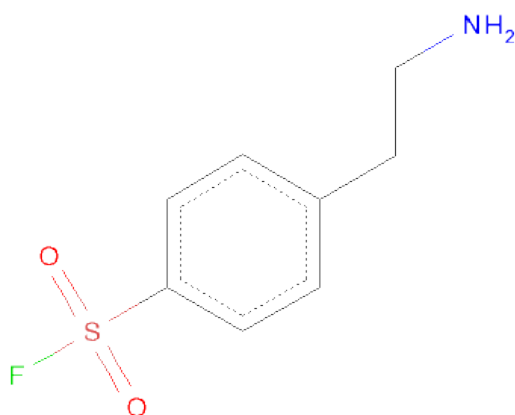
Chain	Residue	Modelled	Actual	Comment	Reference
P	337	SER	ASN	ENGINEERED	UNP Q8T6B1
Q	-7	MET	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-6	ALA	-	CLONING ARTIFACT	UNP Q8T6B1
Q	-5	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-4	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-3	HIS	-	EXPRESSION TAG	UNP Q8T6B1
Q	-2	HIS	-	EXPRESSION TAG	UNP 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)BENZENESULFONYLFLUORIDE (three-letter code: AES) (formula: C₈H₁₀FNO₂S).



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

- Molecule 4 is water.

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

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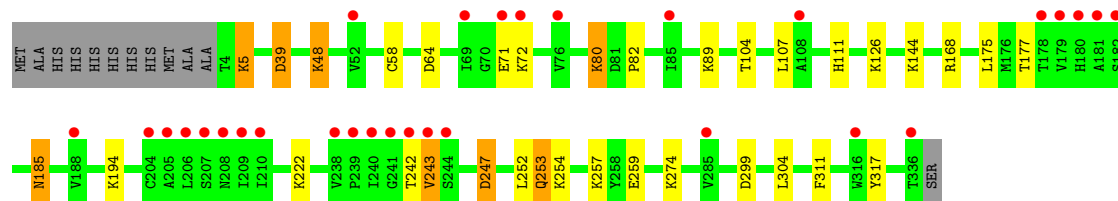
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	49	Total	O	0	0
			49	49		
4	R	55	Total	O	0	0
			55	55		

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.

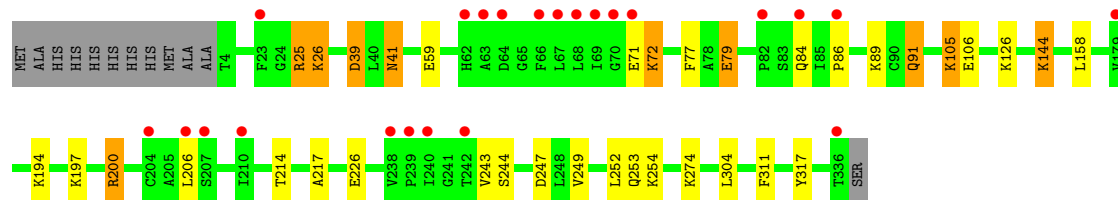
- Molecule 1: glyceraldehyde-3-phosphatedehydrogenase

Chain O: 



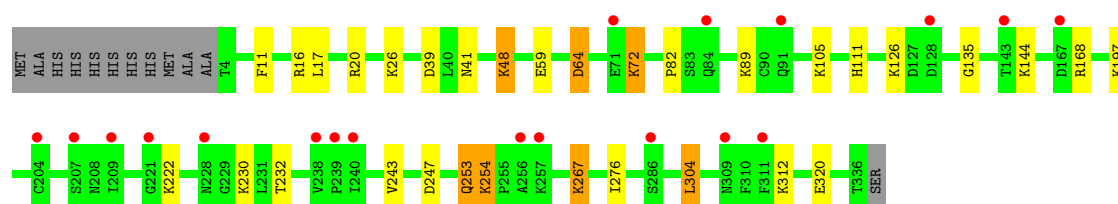
- Molecule 1: glyceraldehyde-3-phosphatedehydrogenase

Chain P: 



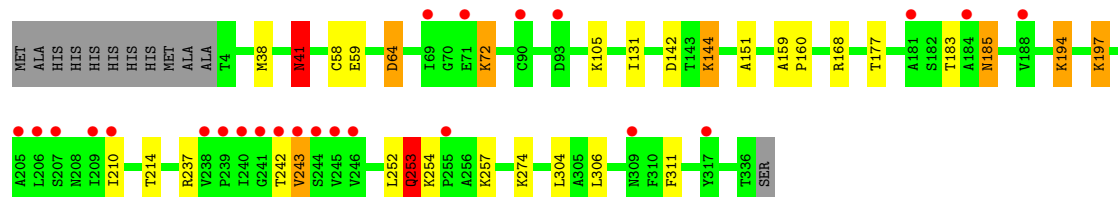
- Molecule 1: glyceraldehyde-3-phosphatedehydrogenase

Chain Q: 



- Molecule 1: glyceraldehyde-3-phosphatedehydrogenase

Chain R: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.217 0.188 , 0.189	Depositor DCC
R_{free} test set	2115 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42822 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10631	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

All (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
1	R	105	LYS	CD-CE	35.09	2.38	1.51
1	O	71	GLU	CA-CB	-33.78	0.79	1.53
1	P	71	GLU	CG-CD	-30.20	1.06	1.51
1	O	48	LYS	CD-CE	-28.92	0.79	1.51
1	R	194	LYS	CB-CG	27.55	2.27	1.52
1	O	64	ASP	CA-CB	24.50	2.07	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	144	LYS	CB-CG	23.95	2.17	1.52
1	P	105	LYS	CB-CG	-22.59	0.91	1.52
1	O	144	LYS	CA-CB	22.33	2.03	1.53
1	P	72	LYS	CG-CD	-20.31	0.83	1.52
1	P	41	ASN	CB-CG	20.16	1.97	1.51
1	Q	72	LYS	CG-CD	-19.23	0.87	1.52
1	O	5	LYS	CB-CG	-19.21	1.00	1.52
1	Q	267	LYS	CB-CG	-19.10	1.00	1.52
1	R	72	LYS	CG-CD	-18.94	0.88	1.52
1	R	41	ASN	CB-CG	-18.45	1.08	1.51
1	R	254	LYS	CB-CG	18.39	2.02	1.52
1	Q	39	ASP	CB-CG	-17.69	1.14	1.51
1	Q	41	ASN	CB-CG	-16.61	1.12	1.51
1	P	226	GLU	CG-CD	-16.55	1.27	1.51
1	Q	26	LYS	CB-CG	-15.75	1.10	1.52
1	O	89	LYS	CD-CE	15.40	1.89	1.51
1	Q	144	LYS	CB-CG	-15.17	1.11	1.52
1	R	59	GLU	CB-CG	14.59	1.79	1.52
1	O	194	LYS	CB-CG	-12.91	1.17	1.52
1	O	126	LYS	CG-CD	-12.57	1.09	1.52
1	O	254	LYS	CD-CE	-12.27	1.20	1.51
1	R	144	LYS	CG-CD	-11.99	1.11	1.52
1	O	194	LYS	CG-CD	-11.65	1.12	1.52
1	O	39	ASP	CB-CG	-11.52	1.27	1.51
1	O	72	LYS	CG-CD	11.45	1.91	1.52
1	P	26	LYS	CB-CG	-11.14	1.22	1.52
1	O	274	LYS	CG-CD	-10.93	1.15	1.52
1	Q	64	ASP	CA-CB	-10.49	1.30	1.53
1	P	194	LYS	CG-CD	-10.26	1.17	1.52
1	P	126	LYS	CD-CE	10.19	1.76	1.51
1	P	126	LYS	CG-CD	-9.54	1.20	1.52
1	O	257	LYS	CG-CD	-9.23	1.21	1.52
1	Q	197	LYS	CB-CG	-9.01	1.28	1.52
1	O	253	GLN	CG-CD	-8.57	1.31	1.51
1	R	197	LYS	CB-CG	-8.45	1.29	1.52
1	O	259	GLU	CG-CD	-8.32	1.39	1.51
1	Q	144	LYS	CD-CE	8.27	1.72	1.51
1	P	89	LYS	CB-CG	7.74	1.73	1.52
1	R	257	LYS	CG-CD	7.60	1.78	1.52
1	O	80	LYS	CB-CG	-7.58	1.32	1.52
1	Q	253	GLN	CG-CD	7.57	1.68	1.51
1	P	106	GLU	CG-CD	-6.66	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	254	LYS	CD-CE	6.49	1.67	1.51
1	P	254	LYS	CD-CE	6.07	1.66	1.51
1	P	274	LYS	CG-CD	-5.99	1.32	1.52
1	R	64	ASP	CA-CB	-5.98	1.40	1.53
1	Q	48	LYS	CD-CE	5.86	1.65	1.51
1	P	71	GLU	CB-CG	5.82	1.63	1.52
1	Q	105	LYS	CB-CG	5.37	1.67	1.52

All (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
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
1	O	80	LYS	CA-CB-CG	23.71	165.56	113.40
1	R	253	GLN	CG-CD-OE1	-21.82	77.96	121.60
1	O	48	LYS	CD-CE-NZ	21.46	161.06	111.70
1	P	25	ARG	CB-CG-CD	21.16	166.62	111.60
1	Q	41	ASN	CA-CB-CG	20.18	157.80	113.40
1	O	64	ASP	CA-CB-CG	-19.08	71.42	113.40
1	R	253	GLN	CB-CG-CD	-18.84	62.60	111.60
1	Q	72	LYS	CB-CG-CD	18.71	160.24	111.60
1	P	39	ASP	CB-CG-OD1	17.09	133.69	118.30
1	P	41	ASN	CA-CB-CG	-16.34	77.45	113.40
1	P	72	LYS	CB-CG-CD	16.25	153.86	111.60
1	P	39	ASP	CB-CG-OD2	-15.70	104.17	118.30
1	Q	39	ASP	CB-CG-OD1	-14.70	105.08	118.30
1	R	253	GLN	CG-CD-NE2	14.58	151.69	116.70
1	Q	39	ASP	CB-CG-OD2	14.51	131.36	118.30
1	R	197	LYS	CA-CB-CG	13.83	143.83	113.40
1	Q	41	ASN	CB-CG-OD1	-13.60	94.41	121.60
1	R	254	LYS	CA-CB-CG	13.59	143.29	113.40
1	R	257	LYS	CB-CG-CD	-13.05	77.67	111.60
1	R	144	LYS	CA-CB-CG	-13.03	84.73	113.40
1	R	41	ASN	CA-CB-CG	12.52	140.94	113.40
1	P	226	GLU	CB-CG-CD	12.36	147.57	114.20
1	Q	72	LYS	CG-CD-CE	11.77	147.22	111.90
1	R	105	LYS	CG-CD-CE	-11.21	78.27	111.90
1	P	71	GLU	CA-CB-CG	11.09	137.81	113.40
1	O	247	ASP	CA-CB-CG	10.91	137.40	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	41	ASN	CB-CG-ND2	10.89	142.83	116.70
1	O	64	ASP	N-CA-CB	10.84	130.11	110.60
1	R	64	ASP	CB-CA-C	10.61	131.61	110.40
1	O	72	LYS	CG-CD-CE	10.60	143.70	111.90
1	R	41	ASN	CB-CG-ND2	-10.39	91.77	116.70
1	O	194	LYS	CB-CG-CD	10.35	138.51	111.60
1	Q	254	LYS	CB-CG-CD	-10.34	84.71	111.60
1	R	72	LYS	CG-CD-CE	10.20	142.49	111.90
1	Q	197	LYS	CA-CB-CG	-10.13	91.11	113.40
1	P	144	LYS	CD-CE-NZ	-10.06	88.55	111.70
1	O	253	GLN	CB-CG-CD	9.78	137.04	111.60
1	P	226	GLU	CG-CD-OE1	-9.77	98.77	118.30
1	O	257	LYS	CB-CG-CD	9.71	136.85	111.60
1	R	197	LYS	CB-CG-CD	9.47	136.22	111.60
1	O	247	ASP	CB-CG-OD1	-9.40	109.84	118.30
1	P	106	GLU	CB-CG-CD	9.39	139.56	114.20
1	Q	254	LYS	CA-CB-CG	-9.38	92.77	113.40
1	Q	253	GLN	CB-CG-CD	-9.37	87.25	111.60
1	Q	222	LYS	CG-CD-CE	-9.15	84.44	111.90
1	R	257	LYS	CG-CD-CE	-9.09	84.63	111.90
1	Q	64	ASP	CB-CA-C	9.03	128.46	110.40
1	Q	197	LYS	CB-CG-CD	-8.94	88.36	111.60
1	P	194	LYS	CB-CG-CD	8.94	134.84	111.60
1	R	64	ASP	CA-CB-CG	8.77	132.68	113.40
1	R	105	LYS	CD-CE-NZ	8.69	131.69	111.70
1	R	274	LYS	CB-CG-CD	8.62	134.00	111.60
1	Q	105	LYS	CA-CB-CG	-8.58	94.52	113.40
1	O	247	ASP	CB-CG-OD2	8.36	125.82	118.30
1	O	126	LYS	CB-CG-CD	-8.34	89.92	111.60
1	Q	267	LYS	CB-CG-CD	-8.26	90.14	111.60
1	Q	26	LYS	CB-CG-CD	8.19	132.88	111.60
1	P	91	GLN	N-CA-CB	-8.16	95.91	110.60
1	P	72	LYS	CG-CD-CE	8.10	136.20	111.90
1	Q	39	ASP	CA-CB-CG	8.10	131.22	113.40
1	P	226	GLU	CG-CD-OE2	8.08	134.46	118.30
1	P	41	ASN	CB-CG-OD1	-7.96	105.68	121.60
1	P	274	LYS	CB-CG-CD	-7.93	90.98	111.60
1	P	91	GLN	CB-CA-C	7.77	125.94	110.40
1	R	254	LYS	CB-CG-CD	7.59	131.33	111.60
1	P	254	LYS	CB-CG-CD	7.55	131.23	111.60
1	Q	105	LYS	CB-CG-CD	-7.52	92.05	111.60
1	O	126	LYS	CG-CD-CE	-7.43	89.60	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	71	GLU	CG-CD-OE2	7.33	132.96	118.30
1	R	41	ASN	CB-CG-OD1	7.29	136.18	121.60
1	P	126	LYS	CB-CG-CD	7.01	129.83	111.60
1	P	26	LYS	CB-CG-CD	6.99	129.78	111.60
1	P	106	GLU	CG-CD-OE2	6.94	132.18	118.30
1	P	71	GLU	CG-CD-OE1	-6.88	104.55	118.30
1	P	253	GLN	CB-CG-CD	6.80	129.29	111.60
1	P	106	GLU	CG-CD-OE1	-6.69	104.91	118.30
1	Q	126	LYS	CG-CD-CE	6.68	131.93	111.90
1	P	274	LYS	CG-CD-CE	-6.64	91.97	111.90
1	O	259	GLU	CB-CG-CD	6.61	132.04	114.20
1	P	105	LYS	CA-CB-CG	6.45	127.58	113.40
1	Q	64	ASP	CA-CB-CG	6.21	127.06	113.40
1	O	144	LYS	CB-CA-C	-6.02	98.37	110.40
1	R	274	LYS	CG-CD-CE	6.01	129.92	111.90
1	P	253	GLN	CG-CD-OE1	-5.51	110.57	121.60
1	O	254	LYS	CD-CE-NZ	5.38	124.06	111.70
1	O	89	LYS	CD-CE-NZ	-5.31	99.49	111.70
1	Q	48	LYS	CG-CD-CE	5.28	127.74	111.90
1	Q	126	LYS	CB-CG-CD	5.14	124.97	111.60
1	P	200	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	P	126	LYS	CG-CD-CE	-5.06	96.72	111.90

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (33) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:P:79:GLU:HG2	1:P:84:GLN:HB2	1.90	0.53
1:P:252:LEU:HD12	1:P:311:PHE:CE1	2.44	0.53
1:O:185:ASN:H	1:O:185:ASN:HD22	1.57	0.52
1:O:104:THR:HG22	1:O:107:LEU:HD12	1.92	0.50
1:O:39:ASP:HB2	4:O:654:HOH:O	2.13	0.48
1:Q:20:ARG:HB2	4:Q:824:HOH:O	2.12	0.48
1:R:159:ALA:HB3	1:R:160:PRO:HD3	1.95	0.48
1:O:242:THR:HG23	1:O:243:VAL:HG23	1.96	0.47
1:Q:11:PHE:CE2	1:Q:16:ARG:HG2	2.50	0.47
1:R:131:ILE:CG2	1:R:151:ALA:HB2	2.45	0.46
1:Q:82:PRO:HB3	1:Q:111:HIS:CE1	2.51	0.46
1:Q:135:GLY:HA3	1:Q:276:ILE:HD13	1.99	0.44
1:R:242:THR:HG23	1:R:243:VAL:HG23	1.99	0.44
1:R:142:ASP:HB3	4:R:943:HOH:O	2.16	0.44
1:Q:17:LEU:CD1	1:Q:320:GLU:HB3	2.48	0.44
1:O:82:PRO:HB3	1:O:111:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:175:LEU:HD12	1:P:249:VAL:HG13	2.00	0.43
1:P:206:LEU:HD12	1:P:206:LEU:N	2.33	0.43
1:P:244:SER:HB2	1:P:317:TYR:CZ	2.53	0.43
1:O:252:LEU:HD12	1:O:311:PHE:CE1	2.54	0.42
1:Q:17:LEU:HD13	1:Q:320:GLU:HB3	2.01	0.42
1:P:158:LEU:HD23	1:P:217:ALA:HA	2.00	0.42
1:R:210:ILE:HB	1:R:237:ARG:HB2	2.03	0.41
1:P:77:PHE:CZ	1:P:86:PRO:HG2	2.55	0.41
1:R:252:LEU:HD12	1:R:311:PHE:CE1	2.56	0.41
1:Q:304:LEU:HD23	1:Q:312:LYS:HB3	2.04	0.40
1:Q:232:THR:HG22	1:R:306:LEU:HD13	2.03	0.40
1:O:299:ASP:OD2	1:P:200:ARG:NH2	2.54	0.40

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	Distance(Å)	Clash(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%)	50	73
1	P	331/345 (96%)	311 (94%)	19 (6%)	1 (0%)	50	73
1	Q	331/345 (96%)	310 (94%)	20 (6%)	1 (0%)	50	73
1	R	331/345 (96%)	311 (94%)	18 (5%)	2 (1%)	33	55
All	All	1324/1380 (96%)	1245 (94%)	74 (6%)	5 (0%)	43	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	243	VAL

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Mol	Chain	Res	Type
1	R	243	VAL
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%)	47	73
1	P	277/286 (97%)	267 (96%)	10 (4%)	47	73
1	Q	277/286 (97%)	267 (96%)	10 (4%)	47	73
1	R	277/286 (97%)	266 (96%)	11 (4%)	42	68
All	All	1108/1144 (97%)	1067 (96%)	41 (4%)	45	72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	5	LYS
1	O	48	LYS
1	O	58	CYS
1	O	80	LYS
1	O	168	ARG
1	O	185	ASN
1	O	222	LYS
1	O	247	ASP
1	O	304	LEU
1	O	317	TYR
1	P	25	ARG
1	P	26	LYS
1	P	39	ASP
1	P	72	LYS
1	P	79	GLU
1	P	91	GLN
1	P	105	LYS
1	P	197	LYS

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Mol	Chain	Res	Type
1	P	214	THR
1	P	304	LEU
1	Q	48	LYS
1	Q	59	GLU
1	Q	64	ASP
1	Q	72	LYS
1	Q	89	LYS
1	Q	168	ARG
1	Q	247	ASP
1	Q	254	LYS
1	Q	267	LYS
1	Q	304	LEU
1	R	41	ASN
1	R	58	CYS
1	R	64	ASP
1	R	72	LYS
1	R	144	LYS
1	R	168	ARG
1	R	185	ASN
1	R	194	LYS
1	R	197	LYS
1	R	214	THR
1	R	304	LEU

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 chains 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	-	48,48,48	1.38	4 (8%)	73,73,73	1.69	8 (10%)
3	AES	O	601	-	13,13,13	0.54	0	18,18,18	2.52	3 (16%)
3	AES	P	602	-	13,13,13	0.65	0	18,18,18	2.21	2 (11%)
2	NAD	P	701	-	48,48,48	1.30	3 (6%)	73,73,73	1.68	11 (15%)
2	NAD	Q	801	-	48,48,48	1.47	4 (8%)	73,73,73	1.67	8 (10%)
3	AES	R	603	-	13,13,13	0.62	0	18,18,18	2.63	3 (16%)
2	NAD	R	901	-	48,48,48	1.36	3 (6%)	73,73,73	1.75	9 (12%)

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	-	-	0/30/62/62	0/3/5/5
3	AES	O	601	-	-	0/9/9/9	0/1/1/1
3	AES	P	602	-	-	0/9/9/9	0/1/1/1
2	NAD	P	701	-	-	0/30/62/62	0/3/5/5
2	NAD	Q	801	-	-	0/30/62/62	0/3/5/5
3	AES	R	603	-	-	0/9/9/9	0/1/1/1
2	NAD	R	901	-	-	0/30/62/62	0/3/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	801	NAD	O7N-C7N	7.64	1.42	1.24
2	O	501	NAD	O7N-C7N	7.21	1.41	1.24
2	R	901	NAD	O7N-C7N	7.17	1.41	1.24
2	P	701	NAD	O7N-C7N	6.83	1.40	1.24
2	O	501	NAD	C2A-N3A	3.37	1.38	1.32
2	R	901	NAD	C2A-N3A	3.33	1.38	1.32
2	Q	801	NAD	C2A-N3A	3.32	1.38	1.32
2	P	701	NAD	C2A-N3A	3.28	1.38	1.32
2	Q	801	NAD	C2A-N1A	2.96	1.39	1.33
2	R	901	NAD	C2A-N1A	2.62	1.39	1.33
2	O	501	NAD	C2A-N1A	2.48	1.38	1.33
2	P	701	NAD	C2A-N1A	2.47	1.38	1.33
2	Q	801	NAD	C2N-N1N	2.42	1.38	1.35
2	O	501	NAD	C2N-N1N	2.16	1.38	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	901	NAD	N3A-C2A-N1A	-10.48	119.94	128.71
2	Q	801	NAD	N3A-C2A-N1A	-10.15	120.23	128.71
2	O	501	NAD	N3A-C2A-N1A	-9.80	120.52	128.71
2	P	701	NAD	N3A-C2A-N1A	-9.54	120.74	128.71
3	R	603	AES	O2S-S-C1	-8.65	104.88	111.02
3	P	602	AES	O2S-S-C1	-7.90	105.41	111.02
3	O	601	AES	O1S-S-C1	-7.54	105.66	111.02
3	O	601	AES	O2S-S-C1	-6.50	106.40	111.02
3	R	603	AES	O1S-S-C1	-5.92	106.81	111.02
2	O	501	NAD	O4D-C1D-N1N	5.00	113.06	107.95
2	R	901	NAD	O4D-C1D-N1N	4.80	112.86	107.95
2	Q	801	NAD	O4D-C1D-N1N	4.76	112.83	107.95
2	P	701	NAD	O4B-C1B-N9A	4.16	112.31	108.44
2	P	701	NAD	O4D-C1D-N1N	4.02	112.06	107.95
3	P	602	AES	O1S-S-C1	-3.90	108.25	111.02
2	Q	801	NAD	N3A-C4A-N9A	3.83	132.34	125.43
2	O	501	NAD	N3A-C4A-N9A	3.59	131.91	125.43
2	R	901	NAD	N3A-C4A-N9A	3.49	131.73	125.43
2	P	701	NAD	N3A-C4A-N9A	3.47	131.71	125.43
2	R	901	NAD	C4A-C5A-N7A	-3.22	106.76	109.52
2	P	701	NAD	C4A-C5A-N7A	-3.03	106.92	109.52
2	R	901	NAD	O4B-C1B-N9A	2.89	111.12	108.44
2	O	501	NAD	PN-O3-PA	-2.87	120.63	132.95
2	O	501	NAD	C4A-C5A-N7A	-2.86	107.07	109.52
3	R	603	AES	F-S-C1	2.75	109.00	102.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	601	AES	F-S-C1	2.60	108.65	102.39
2	R	901	NAD	C5A-C4A-N3A	-2.56	120.12	125.70
2	P	701	NAD	N7A-C8A-N9A	-2.44	107.46	114.36
2	O	501	NAD	C5A-C4A-N3A	-2.43	120.41	125.70
2	R	901	NAD	C2A-N3A-C4A	2.41	120.88	114.01
2	P	701	NAD	C5A-C4A-N3A	-2.27	120.75	125.70
2	Q	801	NAD	C5A-C4A-N3A	-2.26	120.78	125.70
2	Q	801	NAD	N7A-C8A-N9A	-2.20	108.14	114.36
2	P	701	NAD	PN-O3-PA	-2.18	123.58	132.95
2	Q	801	NAD	C4A-C5A-N7A	-2.13	107.69	109.52
2	R	901	NAD	C2N-C3N-C4N	2.13	120.73	118.31
2	O	501	NAD	C2A-N3A-C4A	2.13	120.08	114.01
2	Q	801	NAD	PN-O3-PA	-2.13	123.81	132.95
2	O	501	NAD	N7A-C8A-N9A	-2.12	108.35	114.36
2	P	701	NAD	C8A-N7A-C5A	2.09	110.05	103.58
2	P	701	NAD	C3N-C7N-N7N	2.08	120.13	117.77
2	Q	801	NAD	C2A-N3A-C4A	2.07	119.91	114.01
2	R	901	NAD	N7A-C8A-N9A	-2.07	108.52	114.36
2	P	701	NAD	C2A-N3A-C4A	2.01	119.74	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	O	333/345 (96%)	0.52	30 (9%) 10 9	44, 53, 59, 63	17 (5%)
1	P	333/345 (96%)	0.45	23 (6%) 17 16	44, 52, 63, 68	21 (6%)
1	Q	333/345 (96%)	0.52	19 (5%) 23 23	44, 53, 63, 67	17 (5%)
1	R	333/345 (96%)	0.49	24 (7%) 15 15	46, 52, 59, 67	14 (4%)
All	All	1332/1380 (96%)	0.49	96 (7%) 15 15	44, 53, 61, 68	69 (5%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	167	ASP	3.7
1	P	63	ALA	3.6
1	O	240	ILE	3.5
1	O	205	ALA	3.4
1	P	68	LEU	3.2
1	R	255	PRO	3.2
1	P	23	PHE	3.2
1	P	70	GLY	3.1
1	R	69	ILE	3.1
1	Q	240	ILE	3.1
1	P	71	GLU	3.0
1	R	240	ILE	3.0
1	Q	209	ILE	3.0
1	R	71	GLU	3.0
1	P	66	PHE	2.9
1	P	204	CYS	2.9
1	P	69	ILE	2.9
1	O	238	VAL	2.9
1	R	238	VAL	2.9
1	Q	128	ASP	2.8
1	Q	257	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	R	209	ILE	2.8
1	P	240	ILE	2.8
1	O	204	CYS	2.7
1	R	93	ASP	2.7
1	O	206	LEU	2.7
1	P	67	LEU	2.7
1	O	336	THR	2.6
1	R	181	ALA	2.6
1	P	336	THR	2.6
1	R	90	CYS	2.6
1	O	69	ILE	2.6
1	O	285	VAL	2.6
1	P	210	ILE	2.5
1	P	86	PRO	2.5
1	O	85	ILE	2.5
1	O	181	ALA	2.5
1	P	206	LEU	2.5
1	Q	221	GLY	2.5
1	Q	204	CYS	2.4
1	R	245	VAL	2.4
1	O	243	VAL	2.4
1	O	71	GLU	2.4
1	P	82	PRO	2.4
1	Q	207	SER	2.4
1	R	242	THR	2.4
1	O	182	SER	2.4
1	O	210	ILE	2.4
1	R	239	PRO	2.4
1	R	309	ASN	2.4
1	Q	286	SER	2.4
1	Q	256	ALA	2.3
1	O	209	ILE	2.3
1	R	205	ALA	2.3
1	P	62	HIS	2.3
1	R	246	VAL	2.3
1	O	76	VAL	2.3
1	R	206	LEU	2.2
1	R	243	VAL	2.2
1	Q	238	VAL	2.2
1	Q	84	GLN	2.2
1	Q	143	THR	2.2
1	Q	71	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	239	PRO	2.2
1	Q	311	PHE	2.2
1	O	242	THR	2.2
1	R	188	VAL	2.2
1	O	188	VAL	2.2
1	R	317	TYR	2.2
1	O	208	ASN	2.2
1	O	72	LYS	2.2
1	O	241	GLY	2.1
1	P	238	VAL	2.1
1	Q	91	GLN	2.1
1	P	179	VAL	2.1
1	O	244	SER	2.1
1	R	244	SER	2.1
1	O	316	TRP	2.1
1	R	207	SER	2.1
1	O	179	VAL	2.1
1	P	242	THR	2.1
1	O	108	ALA	2.1
1	P	84	GLN	2.1
1	O	239	PRO	2.1
1	P	64	ASP	2.1
1	Q	239	PRO	2.1
1	R	241	GLY	2.1
1	R	210	ILE	2.1
1	O	178	THR	2.0
1	O	52	VAL	2.0
1	R	184	ALA	2.0
1	Q	228	ASN	2.0
1	P	207	SER	2.0
1	Q	309	ASN	2.0
1	O	207	SER	2.0
1	O	180	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	AES	P	602	13/13	0.18	0.17	66,68,75,76	0
3	AES	R	603	13/13	0.21	0.16	60,68,76,79	0
3	AES	O	601	13/13	0.20	-0.07	56,73,83,85	0
2	NAD	Q	801	44/44	0.16	-0.13	55,66,74,75	0
2	NAD	R	901	44/44	0.15	-0.45	44,50,54,54	0
2	NAD	O	501	44/44	0.15	-0.57	41,52,62,64	0
2	NAD	P	701	44/44	0.13	-0.75	42,50,53,55	0

6.5 Other polymers

There are no such residues in this entry.