



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:53 PM GMT

PDB ID : 2X5J  
Title : CRYSTAL STRUCTURE OF THE APOFORM OF THE D-ERYTHROSE-4-PHOSPHATEDEHYDROGENASE FROM E. COLI  
Authors : Moniot, S.; Didierjean, C.; Boschi-Muller, S.; Branlant, G.; Corbier, C.  
Deposited on : 2010-02-09  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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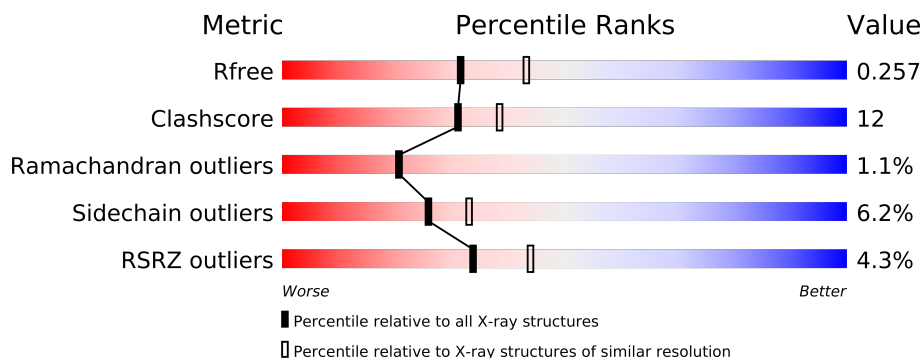
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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	339	
1	P	339	
1	Q	339	
1	R	339	

## 2 Entry composition

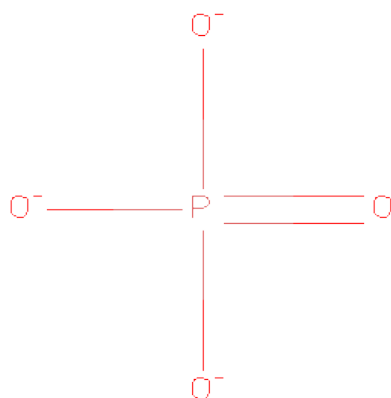
There are 3 unique types of molecules in this entry. The entry contains 10801 atoms, of which 0 are hydrogen and 0 are deuterium.

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 D-ERYTHROSE-4-PHOSPHATEDEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	324	Total	C	N	O	S	0	0	0
			2499	1568	455	468	8			
1	P	328	Total	C	N	O	S	0	0	0
			2526	1585	461	472	8			
1	Q	328	Total	C	N	O	S	0	16	0
			2645	1655	486	497	7			
1	R	330	Total	C	N	O	S	0	3	0
			2572	1613	472	479	8			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

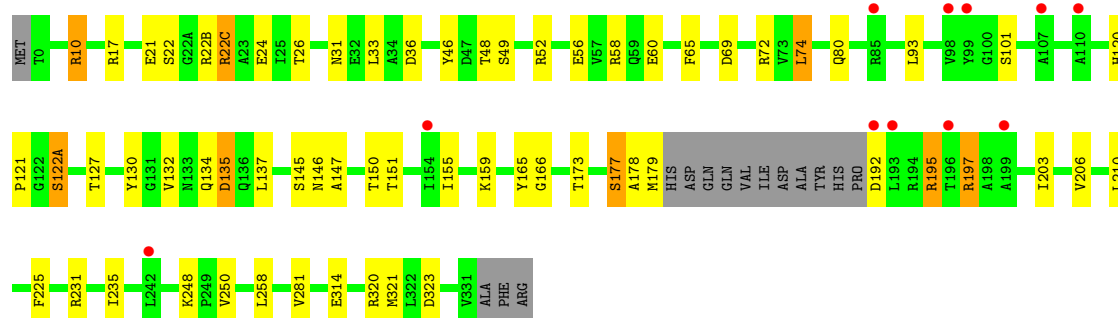
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	136	Total	O	0	0
			136	136		
3	P	109	Total	O	0	0
			109	109		
3	Q	146	Total	O	0	0
			146	146		
3	R	148	Total	O	0	0
			148	148		

### 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.

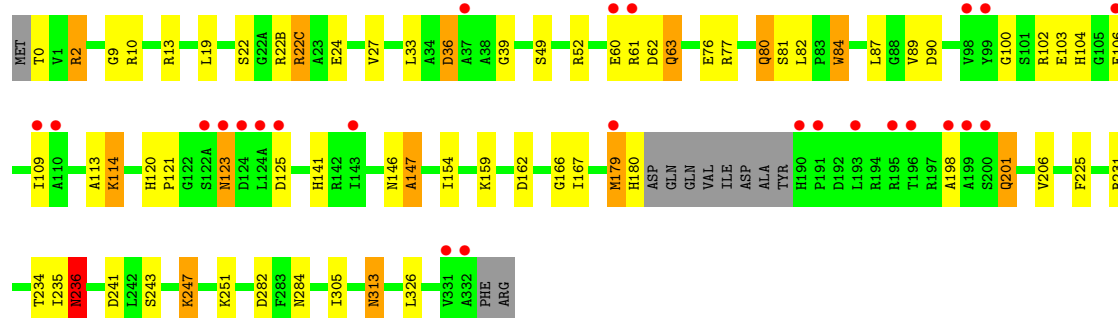
#### • Molecule 1: D-ERYTHROSE-4-PHOSPHATEDEHYDROGENASE

Chain O: 



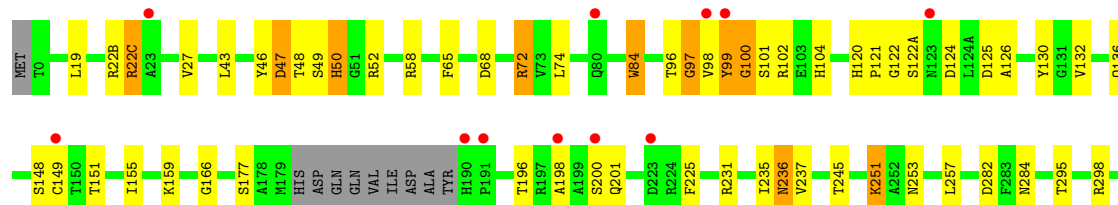
#### • Molecule 1: D-ERYTHROSE-4-PHOSPHATEDEHYDROGENASE

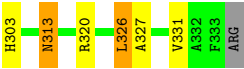
Chain P: 



#### • Molecule 1: D-ERYTHROSE-4-PHOSPHATEDEHYDROGENASE

Chain Q: 





● Molecule 1: D-ERYTHROSE-4-PHOSPHATEDEHYDROGENASE

Chain R:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.30Å 110.70Å 138.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.30 34.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.50-2.30) 99.6 (34.50-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.206 , 0.266 0.201 , 0.257	Depositor DCC
$R_{free}$ test set	2958 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59159 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: PO4

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	0.70	0/2543	0.76	1/3457 (0.0%)
1	P	0.67	0/2572	0.73	1/3498 (0.0%)
1	Q	0.66	0/2694	0.71	1/3665 (0.0%)
1	R	0.70	0/2619	0.75	2/3561 (0.1%)
All	All	0.68	0/10428	0.74	5/14181 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	163	ASP	CB-CG-OD1	5.82	123.54	118.30
1	O	197	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	R	194	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	P	236	ASN	N-CA-C	5.20	125.05	111.00
1	Q	326	LEU	CA-CB-CG	-5.20	103.35	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2499	0	2496	48	0
1	P	2526	0	2517	64	0
1	Q	2645	0	2611	89	0
1	R	2572	0	2561	54	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	1	0
3	O	136	0	0	3	0
3	P	109	0	0	3	0
3	Q	146	0	0	7	0
3	R	148	0	0	7	0
All	All	10801	0	10185	239	0

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 12.

All (239) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:96[B]:THR:HG22	1:Q:98[B]:VAL:CG2	1.65	1.25
1:Q:96[B]:THR:O	1:Q:98[B]:VAL:HG22	1.38	1.22
1:Q:97[A]:GLY:O	1:Q:98[A]:VAL:O	1.60	1.20
1:Q:97[A]:GLY:HA2	1:Q:120[A]:HIS:CE1	1.81	1.16
1:Q:22(B)[B]:ARG:HG2	1:Q:22(B)[B]:ARG:HH11	1.03	1.15
1:Q:96[B]:THR:CG2	1:Q:98[B]:VAL:CG2	2.26	1.11
1:O:206:VAL:HG11	1:O:231:ARG:HD3	1.12	1.11
1:Q:96[B]:THR:HG22	1:Q:98[B]:VAL:HG22	1.24	1.08
1:O:206:VAL:CG1	1:O:231:ARG:HD3	1.90	1.00
1:R:331:VAL:O	1:R:331:VAL:HG13	1.60	0.97
1:P:179:MET:HG2	1:P:180:HIS:H	1.26	0.97
1:O:150:THR:HG22	1:O:210:LEU:HD13	1.45	0.96
1:Q:96[B]:THR:CG2	1:Q:98[B]:VAL:HG22	1.95	0.94
1:Q:22(B)[B]:ARG:CG	1:Q:22(B)[B]:ARG:HH11	1.81	0.93
1:Q:22(B)[B]:ARG:HG2	1:Q:22(B)[B]:ARG:NH1	1.83	0.91
1:Q:96[B]:THR:HG22	1:Q:98[B]:VAL:HG21	1.51	0.91
1:Q:298:ARG:HG2	1:R:226:GLU:HB3	1.52	0.90
1:P:179:MET:HG2	1:P:180:HIS:N	1.83	0.90
1:P:198:ALA:HB3	1:P:201:GLN:OE1	1.72	0.89
1:P:120:HIS:HB2	1:P:121:PRO:HD2	1.56	0.87
1:O:206:VAL:HG11	1:O:231:ARG:CD	2.01	0.84
1:P:201:GLN:HG3	1:Q:48[A]:THR:CG2	2.10	0.81
1:P:61:ARG:HB2	1:P:61:ARG:CZ	2.11	0.81
1:Q:132:VAL:HG13	1:Q:159:LYS:HD3	1.61	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:96[B]:THR:O	1:Q:98[B]:VAL:CG2	2.28	0.80
1:O:151:THR:CG2	1:O:155:ILE:HD12	2.12	0.78
1:R:121:PRO:HB3	1:R:216[B]:ARG:HH22	1.46	0.78
1:R:33:LEU:O	1:R:34:ALA:CB	2.30	0.77
1:O:132:VAL:HG13	1:O:159:LYS:HD2	1.67	0.77
1:R:331:VAL:O	1:R:331:VAL:CG1	2.34	0.76
1:O:151:THR:HG23	1:O:155:ILE:HD12	1.65	0.76
1:R:151:THR:HG23	1:R:155:ILE:HD12	1.68	0.76
1:P:125:ASP:HB3	1:P:141:HIS:HD2	1.51	0.76
1:P:146:ASN:O	1:P:147:ALA:HB3	1.86	0.75
1:R:330:THR:HG22	1:R:331:VAL:N	2.03	0.74
1:P:179:MET:CG	1:P:180:HIS:N	2.49	0.74
1:Q:96[B]:THR:CG2	1:Q:98[B]:VAL:HG21	2.10	0.73
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.24	0.73
1:P:236:ASN:ND2	1:P:284:ASN:OD1	2.22	0.72
1:Q:58:ARG:HB3	1:Q:65:PHE:HB2	1.72	0.72
1:Q:46[B]:TYR:O	1:Q:47[B]:ASP:HB3	1.89	0.72
1:P:206:VAL:HG11	1:P:231:ARG:HD3	1.72	0.71
1:R:48:THR:O	1:R:49:SER:HB3	1.91	0.70
1:Q:99[A]:TYR:HD2	1:Q:99[A]:TYR:H	1.39	0.70
1:R:36:ASP:OD2	1:R:36:ASP:C	2.30	0.70
1:O:46:TYR:HE1	1:O:52:ARG:HE	1.40	0.70
1:Q:298:ARG:HG2	1:R:226:GLU:CB	2.20	0.69
1:Q:198:ALA:O	1:Q:201:GLN:NE2	2.25	0.69
1:Q:102:ARG:NH1	1:Q:125:ASP:OD2	2.23	0.69
1:P:76:GLU:HG2	1:P:81:SER:OG	1.92	0.69
1:O:151:THR:HG23	1:O:155:ILE:CD1	2.22	0.68
1:Q:50[B]:HIS:CE1	3:Q:2022:HOH:O	2.47	0.67
1:Q:46[B]:TYR:O	1:Q:47[B]:ASP:CB	2.42	0.67
1:Q:97[A]:GLY:HA2	1:Q:120[A]:HIS:ND1	2.10	0.66
1:Q:97[A]:GLY:O	1:Q:98[A]:VAL:C	2.34	0.66
1:P:201:GLN:HG2	3:Q:2019:HOH:O	1.96	0.66
1:R:48:THR:CG2	3:R:2011:HOH:O	2.43	0.66
1:Q:236[B]:ASN:ND2	1:Q:284:ASN:OD1	2.23	0.66
1:Q:100[A]:GLY:H	1:Q:122:GLY:HA2	1.60	0.66
1:Q:327:ALA:O	1:Q:331:VAL:HG22	1.96	0.66
1:Q:251:LYS:HG3	1:Q:253:ASN:OD1	1.95	0.66
1:Q:99[B]:TYR:O	3:Q:2059:HOH:O	2.02	0.65
1:R:51:GLY:HA2	3:R:2031:HOH:O	1.96	0.65
1:Q:96[B]:THR:O	1:Q:98[B]:VAL:N	2.29	0.65
1:R:36:ASP:OD2	1:R:37:ALA:N	2.30	0.65
1:R:330:THR:HG22	1:R:331:VAL:H	1.62	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:36:ASP:OD2	1:R:38:ALA:N	2.29	0.65
1:O:17:ARG:O	1:O:21:GLU:HG3	1.97	0.64
1:Q:96[B]:THR:C	1:Q:98[B]:VAL:HG22	2.15	0.64
1:Q:282:ASP:OD1	1:R:197:ARG:NH2	2.28	0.64
1:P:313:ASN:HD22	1:P:313:ASN:H	1.44	0.64
1:Q:50[B]:HIS:CG	1:Q:50[B]:HIS:O	2.51	0.64
1:O:101:SER:HA	1:O:122(A):SER:HB2	1.80	0.63
1:P:201:GLN:CG	1:Q:48[A]:THR:HG21	2.28	0.63
1:O:197:ARG:HH22	1:P:282:ASP:CG	2.01	0.62
1:O:192:ASP:HB2	1:O:195:ARG:HD3	1.81	0.62
1:Q:96[B]:THR:CB	1:Q:98[B]:VAL:HG22	2.29	0.62
1:R:33:LEU:O	1:R:34:ALA:HB3	2.00	0.62
1:P:49:SER:HB3	1:P:236:ASN:ND2	2.14	0.62
1:P:235:ILE:HD12	3:P:2096:HOH:O	1.98	0.62
1:Q:96[B]:THR:HG22	1:Q:96[B]:THR:O	1.98	0.61
1:P:313:ASN:H	1:P:313:ASN:ND2	1.98	0.61
1:R:58:ARG:HG3	1:R:65:PHE:HB2	1.83	0.61
3:O:2124:HOH:O	1:Q:52[A]:ARG:HD2	2.01	0.60
1:Q:22(C):ARG:O	1:Q:22(C):ARG:HG3	2.01	0.60
1:Q:99[B]:TYR:O	1:Q:120[B]:HIS:NE2	2.34	0.59
1:R:151:THR:CG2	1:R:155:ILE:HD12	2.32	0.59
1:O:177:SER:HB3	1:O:235:ILE:O	2.02	0.59
1:Q:96[B]:THR:CB	1:Q:98[B]:VAL:CG2	2.81	0.59
1:P:125:ASP:HB3	1:P:141:HIS:CD2	2.37	0.59
1:Q:282:ASP:CG	1:R:197:ARG:HH22	2.05	0.59
1:O:197:ARG:NH2	1:P:282:ASP:OD1	2.36	0.59
1:Q:125:ASP:O	1:Q:126:ALA:HB2	2.03	0.58
1:P:201:GLN:CG	1:Q:48[A]:THR:CG2	2.80	0.58
1:R:151:THR:HG21	1:R:216[B]:ARG:HH11	1.67	0.58
1:Q:46[B]:TYR:HE1	1:Q:52[B]:ARG:NE	2.01	0.58
1:Q:96[B]:THR:C	1:Q:98[B]:VAL:N	2.56	0.58
1:P:89:VAL:O	1:P:114:LYS:HD3	2.03	0.58
1:Q:245:THR:HA	1:Q:303:HIS:O	2.03	0.58
1:Q:97[A]:GLY:CA	1:Q:120[A]:HIS:CE1	2.73	0.57
1:P:201:GLN:OE1	1:Q:48[A]:THR:HG21	2.04	0.57
1:R:220:GLN:O	1:R:224:ARG:NH2	2.32	0.57
1:P:201:GLN:CD	1:Q:48[A]:THR:HG21	2.25	0.57
1:R:48:THR:O	1:R:49:SER:CB	2.53	0.57
1:P:235:ILE:CD1	3:P:2096:HOH:O	2.51	0.56
1:O:60:GLU:HB3	1:O:65:PHE:HE1	1.70	0.56
1:Q:96[B]:THR:HG21	1:Q:98[B]:VAL:CG2	2.32	0.56
1:P:236:ASN:OD1	1:P:236:ASN:N	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:46[B]:TYR:CE1	1:Q:52[B]:ARG:NE	2.72	0.56
1:P:61:ARG:CZ	1:P:61:ARG:CB	2.82	0.56
1:O:165:TYR:HA	1:O:248:LYS:HD3	1.87	0.56
1:P:60:GLU:O	1:P:61:ARG:HB2	2.06	0.56
1:R:82:LEU:O	1:R:111:ALA:HB1	2.06	0.55
1:R:48:THR:HG21	3:R:2011:HOH:O	2.06	0.55
1:O:258:LEU:HD22	3:O:2108:HOH:O	2.06	0.55
1:O:48:THR:HG21	1:R:198:ALA:HB3	1.87	0.55
1:R:130:TYR:HB3	1:R:320:ARG:HD3	1.88	0.55
1:O:150:THR:HG22	1:O:210:LEU:CD1	2.29	0.54
1:R:330:THR:CG2	1:R:331:VAL:N	2.70	0.54
1:R:33:LEU:O	1:R:34:ALA:HB2	2.06	0.54
1:Q:151:THR:HG23	1:Q:155:ILE:HG13	1.89	0.54
1:P:61:ARG:NH1	1:P:62:ASP:OD2	2.40	0.54
1:R:194:ARG:HB2	1:R:194:ARG:HH11	1.73	0.54
1:Q:48[A]:THR:CG2	3:Q:2019:HOH:O	2.55	0.54
1:Q:99[A]:TYR:N	1:Q:99[A]:TYR:CD2	2.73	0.53
1:Q:22(B)[B]:ARG:NH1	1:Q:22(B)[B]:ARG:CG	2.52	0.53
1:R:251:LYS:HE2	1:R:253:ASN:OD1	2.09	0.52
1:P:9:GLY:O	1:P:13:ARG:HG3	2.10	0.52
1:O:22(B):ARG:NH1	1:O:323:ASP:OD1	2.43	0.52
1:Q:96[B]:THR:C	1:Q:98[B]:VAL:H	2.13	0.52
1:P:123:ASN:OD1	1:P:123:ASN:N	2.34	0.51
1:P:36:ASP:OD1	1:P:39:GLY:N	2.30	0.51
1:R:151:THR:HG23	1:R:155:ILE:CD1	2.41	0.50
1:P:22:SER:HB2	3:P:2016:HOH:O	2.11	0.50
1:O:281:VAL:HG11	1:Q:48[A]:THR:HG23	1.93	0.50
1:P:36:ASP:C	1:P:36:ASP:OD1	2.48	0.50
1:P:36:ASP:O	1:P:36:ASP:OD1	2.30	0.50
1:P:22(C):ARG:O	1:P:22(C):ARG:NE	2.45	0.50
1:O:150:THR:CG2	1:O:210:LEU:HD13	2.31	0.50
1:Q:151:THR:CG2	1:Q:155:ILE:HG13	2.41	0.50
1:P:114:LYS:N	1:P:114:LYS:HD2	2.27	0.49
1:P:109:ILE:HA	1:P:113:ALA:O	2.11	0.49
1:Q:72:ARG:HD2	1:Q:74:LEU:HD21	1.93	0.49
1:Q:313:ASN:H	1:Q:313:ASN:ND2	2.09	0.49
1:Q:46[B]:TYR:OH	1:Q:52[B]:ARG:NH2	2.44	0.49
1:Q:99[B]:TYR:O	1:Q:120[B]:HIS:CD2	2.66	0.49
1:O:22(C):ARG:NH2	1:O:26:THR:HB	2.27	0.49
1:O:151:THR:HG22	1:O:155:ILE:HD12	1.95	0.48
1:P:114:LYS:CD	1:P:114:LYS:H	2.26	0.48
1:R:98:VAL:HG23	1:R:99:TYR:N	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:49[B]:SER:O	1:Q:50[B]:HIS:CB	2.62	0.48
1:Q:235:ILE:O	1:Q:237:VAL:N	2.47	0.47
1:Q:46[B]:TYR:HE1	1:Q:52[B]:ARG:CZ	2.27	0.47
1:R:2:ARG:NH1	1:R:87:LEU:O	2.37	0.47
1:Q:84:TRP:CE3	1:Q:84:TRP:HA	2.49	0.47
1:P:201:GLN:HG3	1:Q:48[A]:THR:HG23	1.92	0.47
1:P:146:ASN:O	1:P:147:ALA:CB	2.53	0.46
1:P:102:ARG:O	1:P:106:GLU:HG2	2.16	0.46
1:R:149:CYS:HB3	1:R:313:ASN:HB2	1.96	0.46
1:R:192:ASP:C	1:R:192:ASP:OD2	2.54	0.46
1:P:61:ARG:HH22	1:P:63:GLN:HG3	1.81	0.46
1:O:31:ASN:HB2	1:O:74:LEU:HD12	1.97	0.46
1:R:9:GLY:O	1:R:10:ARG:C	2.54	0.46
1:R:213:GLY:O	1:R:216[B]:ARG:HG3	2.15	0.46
1:P:206:VAL:HG11	1:P:231:ARG:CD	2.45	0.46
1:R:138:ARG:H	1:R:141:HIS:CE1	2.33	0.46
1:R:92:VAL:HG13	1:R:116:VAL:HG13	1.96	0.46
1:Q:177:SER:CB	1:Q:236[A]:ASN:HA	2.45	0.46
1:R:82:LEU:HD13	1:R:84:TRP:CZ2	2.50	0.46
1:O:10:ARG:HB3	1:O:10:ARG:HH11	1.80	0.46
1:Q:46[B]:TYR:CD1	1:Q:52[B]:ARG:HG2	2.51	0.46
1:P:2:ARG:NH1	1:P:87:LEU:O	2.46	0.46
1:Q:84:TRP:HE3	1:Q:84:TRP:HA	1.80	0.46
1:R:235:ILE:O	1:R:236:ASN:ND2	2.49	0.46
1:O:127:THR:HA	1:O:145:SER:O	2.16	0.46
1:Q:313:ASN:H	1:Q:313:ASN:HD22	1.62	0.45
1:O:130:TYR:HB3	1:O:320:ARG:HD3	1.98	0.45
1:O:235:ILE:HG22	1:R:201:GLN:NE2	2.31	0.45
1:R:307[A]:THR:HG23	3:R:2132:HOH:O	2.16	0.45
1:P:90:ASP:HA	1:P:114:LYS:HD3	1.99	0.45
1:R:84:TRP:HA	1:R:84:TRP:HE3	1.82	0.45
1:Q:72:ARG:NH1	3:Q:2044:HOH:O	2.33	0.45
1:Q:327:ALA:O	1:Q:331:VAL:CG2	2.64	0.45
1:P:243:SER:HA	1:P:305:ILE:O	2.16	0.45
1:P:33:LEU:HD23	1:P:33:LEU:HA	1.83	0.45
1:O:65:PHE:HA	1:O:69:ASP:O	2.17	0.45
1:R:84:TRP:CE3	1:R:84:TRP:HA	2.52	0.45
1:O:120:HIS:HB2	1:O:121:PRO:HD2	1.97	0.45
1:O:135:ASP:OD1	1:O:135:ASP:N	2.40	0.44
1:P:61:ARG:NH1	1:P:61:ARG:CB	2.80	0.44
1:P:162:ASP:HB2	1:P:167:ILE:HD12	2.00	0.44
1:O:146:ASN:O	1:O:147:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:130:TYR:CE2	1:O:323:ASP:HB3	2.52	0.44
1:O:33:LEU:HG	3:O:2019:HOH:O	2.18	0.43
1:O:165:TYR:CE2	1:O:250:VAL:HG11	2.53	0.43
1:Q:149:CYS:HB3	1:Q:313:ASN:HB2	2.00	0.43
1:R:25:ILE:HD11	1:R:326:LEU:HG	2.00	0.43
1:R:216[A]:ARG:HG2	3:R:2094:HOH:O	2.18	0.43
1:Q:101[A]:SER:OG	1:Q:104:HIS:ND1	2.49	0.43
1:Q:295:THR:O	1:Q:298:ARG:NH2	2.52	0.43
1:R:168:GLU:OE2	1:R:247:LYS:HD3	2.18	0.43
1:O:173:THR:OG1	1:P:241:ASP:OD1	2.25	0.43
1:Q:100[B]:GLY:HA3	1:Q:120[B]:HIS:NE2	2.33	0.43
1:R:219:PRO:O	1:R:222:ASN:ND2	2.51	0.43
1:Q:96[B]:THR:HB	1:Q:98[B]:VAL:CG2	2.49	0.43
1:Q:130:TYR:HB3	1:Q:320:ARG:HD3	2.01	0.43
1:O:130:TYR:CZ	1:O:323:ASP:HB3	2.54	0.42
1:P:61:ARG:HB3	1:P:62:ASP:H	1.50	0.42
1:O:235:ILE:H	1:O:235:ILE:HG13	1.60	0.42
1:P:154:ILE:HD12	1:P:154:ILE:HA	1.80	0.42
1:P:103:GLU:HG2	1:P:104:HIS:H	1.84	0.42
1:R:216[A]:ARG:CG	3:R:2094:HOH:O	2.68	0.42
1:P:114:LYS:HD2	1:P:114:LYS:H	1.84	0.42
1:Q:19:LEU:HD22	1:Q:27:VAL:HG23	2.02	0.42
1:R:48:THR:HG22	1:R:48:THR:O	2.20	0.42
1:O:177:SER:HB2	1:O:178:ALA:H	1.58	0.42
1:Q:43:LEU:O	1:Q:46[B]:TYR:O	2.38	0.41
1:Q:251:LYS:CG	1:Q:253:ASN:OD1	2.68	0.41
1:R:313:ASN:H	1:R:313:ASN:ND2	2.18	0.41
1:O:10:ARG:NH1	1:O:314:GLU:OE1	2.53	0.41
1:O:120:HIS:HB2	1:O:121:PRO:CD	2.49	0.41
1:Q:121:PRO:HD3	1:Q:148:SER:HB3	2.01	0.41
2:R:1600:PO4:O4	3:R:2146:HOH:O	2.22	0.41
1:Q:96[B]:THR:HG21	1:Q:98[B]:VAL:HG21	1.97	0.41
1:O:22:SER:OG	1:O:22(B):ARG:HG3	2.20	0.41
1:O:134:GLN:O	1:O:137:LEU:HB2	2.20	0.41
1:O:203:ILE:HG13	1:P:234:THR:HG21	2.02	0.41
1:P:114:LYS:N	1:P:114:LYS:CD	2.83	0.41
1:Q:68:ASP:HA	3:Q:2036:HOH:O	2.20	0.41
1:P:120:HIS:HB2	1:P:121:PRO:CD	2.40	0.41
1:P:247:LYS:HB3	1:P:247:LYS:NZ	2.34	0.41
1:O:132:VAL:HG13	1:O:159:LYS:CD	2.44	0.41
1:P:103:GLU:HG2	1:P:104:HIS:N	2.36	0.41
1:R:120:HIS:HB2	1:R:121:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:46[B]:TYR:CE1	1:Q:52[B]:ARG:HG2	2.55	0.41
1:O:93:LEU:HD23	1:O:321:MET:HG2	2.03	0.41
1:P:19:LEU:HD22	1:P:27:VAL:HG23	2.03	0.40
1:P:80:GLN:HG3	1:P:80:GLN:H	1.64	0.40
1:Q:122(A):SER:HB3	3:Q:2063:HOH:O	2.21	0.40

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	320/339 (94%)	307 (96%)	12 (4%)	1 (0%)	50	60
1	P	324/339 (96%)	305 (94%)	15 (5%)	4 (1%)	19	19
1	Q	340/339 (100%)	304 (89%)	24 (7%)	12 (4%)	6	3
1	R	329/339 (97%)	312 (95%)	15 (5%)	2 (1%)	33	39
All	All	1313/1356 (97%)	1228 (94%)	66 (5%)	19 (1%)	21	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	236	ASN
1	Q	50[A]	HIS
1	Q	50[B]	HIS
1	Q	236[A]	ASN
1	Q	236[B]	ASN
1	R	34	ALA
1	Q	97[A]	GLY
1	Q	97[B]	GLY
1	P	100	GLY
1	Q	47[A]	ASP
1	Q	47[B]	ASP
1	Q	100[A]	GLY
1	Q	100[B]	GLY

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Mol	Chain	Res	Type
1	P	166	GLY
1	Q	124	ASP
1	R	330	THR
1	P	147	ALA
1	Q	166	GLY
1	O	166	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	267/280 (95%)	251 (94%)	16 (6%)	27	35
1	P	269/280 (96%)	247 (92%)	22 (8%)	17	19
1	Q	280/280 (100%)	266 (95%)	14 (5%)	34	45
1	R	273/280 (98%)	257 (94%)	16 (6%)	28	35
All	All	1089/1120 (97%)	1021 (94%)	68 (6%)	26	33

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	10	ARG
1	O	22(C)	ARG
1	O	24	GLU
1	O	36	ASP
1	O	49	SER
1	O	56	GLU
1	O	58	ARG
1	O	72	ARG
1	O	74	LEU
1	O	80	GLN
1	O	122(A)	SER
1	O	135	ASP
1	O	177	SER
1	O	179	MET
1	O	195	ARG
1	O	225	PHE

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Mol	Chain	Res	Type
1	P	0	THR
1	P	2	ARG
1	P	10	ARG
1	P	22(B)	ARG
1	P	22(C)	ARG
1	P	24	GLU
1	P	36	ASP
1	P	52	ARG
1	P	63	GLN
1	P	77	ARG
1	P	80	GLN
1	P	84	TRP
1	P	114	LYS
1	P	123	ASN
1	P	159	LYS
1	P	179	MET
1	P	201	GLN
1	P	225	PHE
1	P	247	LYS
1	P	251	LYS
1	P	313	ASN
1	P	326	LEU
1	Q	22(C)	ARG
1	Q	72	ARG
1	Q	84	TRP
1	Q	99[A]	TYR
1	Q	99[B]	TYR
1	Q	136	GLN
1	Q	196	THR
1	Q	200	SER
1	Q	225	PHE
1	Q	231	ARG
1	Q	251	LYS
1	Q	257	LEU
1	Q	313	ASN
1	Q	326	LEU
1	R	0	THR
1	R	8	PHE
1	R	36	ASP
1	R	45	LYS
1	R	59	GLN
1	R	84	TRP

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Mol	Chain	Res	Type
1	R	142	ARG
1	R	194	ARG
1	R	197	ARG
1	R	200	SER
1	R	215	THR
1	R	216[A]	ARG
1	R	216[B]	ARG
1	R	225	PHE
1	R	236	ASN
1	R	330	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	264	GLN
1	P	313	ASN
1	Q	63	GLN
1	Q	313	ASN
1	R	50	HIS
1	R	176	HIS
1	R	236	ASN
1	R	313	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 ⓘ

4 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	PO4	O	1600	-	4,4,4	0.35	0	6,6,6	0.31	0
2	PO4	P	1600	-	4,4,4	0.24	0	6,6,6	0.30	0
2	PO4	Q	1600	-	4,4,4	0.31	0	6,6,6	0.32	0
2	PO4	R	1600	-	4,4,4	0.40	0	6,6,6	0.32	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
2	PO4	O	1600	-	-	0/0/0/0	0/0/0/0
2	PO4	P	1600	-	-	0/0/0/0	0/0/0/0
2	PO4	Q	1600	-	-	0/0/0/0	0/0/0/0
2	PO4	R	1600	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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, 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	324/339 (95%)	0.16	11 (3%) 43 53	17, 34, 52, 60	0
1	P	328/339 (96%)	0.27	25 (7%) 14 20	18, 34, 57, 68	0
1	Q	328/339 (96%)	0.03	11 (3%) 43 53	17, 28, 49, 78	0
1	R	330/339 (97%)	0.04	9 (2%) 52 62	19, 31, 50, 64	0
All	All	1310/1356 (96%)	0.12	56 (4%) 34 44	17, 31, 53, 78	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	331	VAL	5.6
1	P	191	PRO	4.7
1	Q	99[A]	TYR	4.6
1	Q	191	PRO	4.2
1	P	332	ALA	4.1
1	P	122(A)	SER	4.0
1	P	61	ARG	4.0
1	P	200	SER	3.7
1	R	332	ALA	3.5
1	Q	190	HIS	3.5
1	R	189	TYR	3.4
1	O	199	ALA	3.3
1	O	99	TYR	3.3
1	P	190	HIS	3.2
1	Q	80	GLN	3.1
1	P	199	ALA	3.1
1	P	195	ARG	3.1
1	Q	198	ALA	3.1
1	P	110	ALA	3.0
1	P	125	ASP	3.0
1	R	333	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	99	TYR	3.0
1	P	60	GLU	3.0
1	P	179	MET	2.9
1	O	107	ALA	2.9
1	R	59	GLN	2.9
1	Q	200	SER	2.9
1	P	124(A)	LEU	2.8
1	O	154	ILE	2.7
1	R	50	HIS	2.7
1	O	192	ASP	2.6
1	R	61	ARG	2.6
1	P	37	ALA	2.5
1	R	33	LEU	2.4
1	O	98	VAL	2.4
1	P	123	ASN	2.4
1	P	98	VAL	2.4
1	P	193	LEU	2.4
1	Q	123	ASN	2.3
1	O	196	THR	2.3
1	Q	98[A]	VAL	2.2
1	P	196	THR	2.2
1	O	85	ARG	2.2
1	Q	23	ALA	2.2
1	R	34	ALA	2.1
1	O	242	LEU	2.1
1	P	106	GLU	2.1
1	O	110	ALA	2.1
1	P	109	ILE	2.1
1	P	124	ASP	2.1
1	P	198	ALA	2.1
1	O	193	LEU	2.0
1	P	143	ILE	2.0
1	Q	149	CYS	2.0
1	Q	223	ASP	2.0
1	R	149	CYS	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	Q	1600	5/5	0.18	-	40,40,41,44	5
2	PO4	P	1600	5/5	0.14	-	33,33,34,36	5
2	PO4	R	1600	5/5	0.19	-	33,34,35,35	5
2	PO4	O	1600	5/5	0.18	-	45,45,47,48	5

### 6.5 Other polymers ⓘ

There are no such residues in this entry.