



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:22 PM UTC

PDB ID : 2X5J / pdb_00002x5j
Title : Crystal structure of the Apoform of the D-Erythrose-4-phosphate dehydrogenase 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

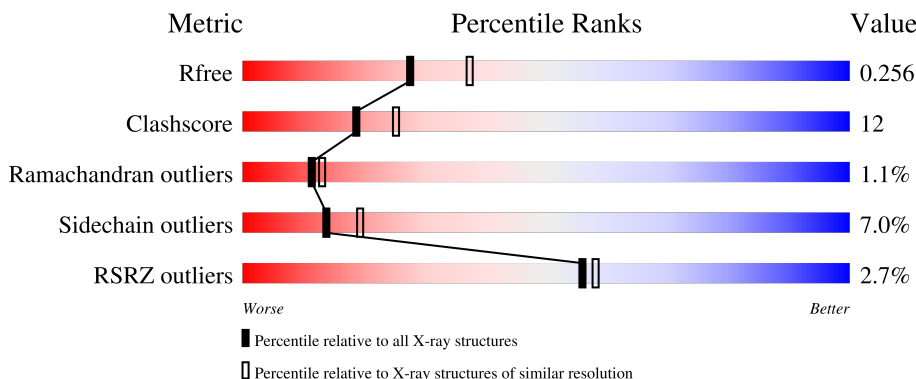
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

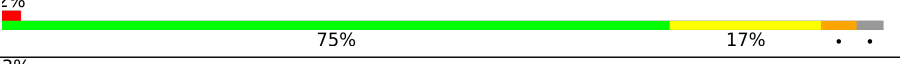
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	339	
1	P	339	
1	Q	339	
1	R	339	

2 Entry composition [i](#)

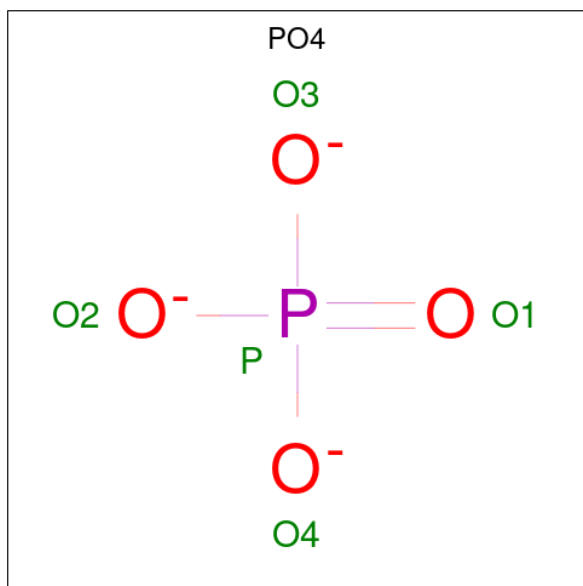
There are 3 unique types of molecules in this entry. The entry contains 10801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE.

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 (CCD ID: PO4) (formula: O₄P).



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		

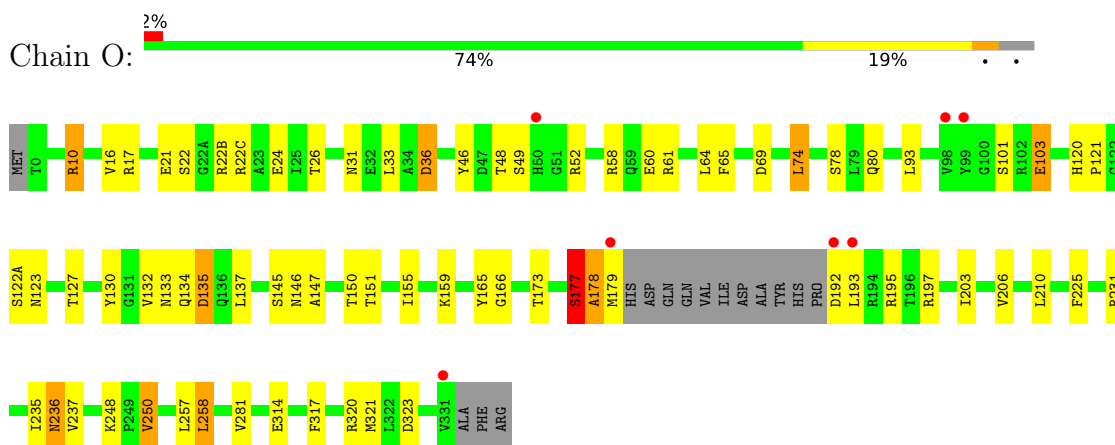
- Molecule 3 is water.

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		

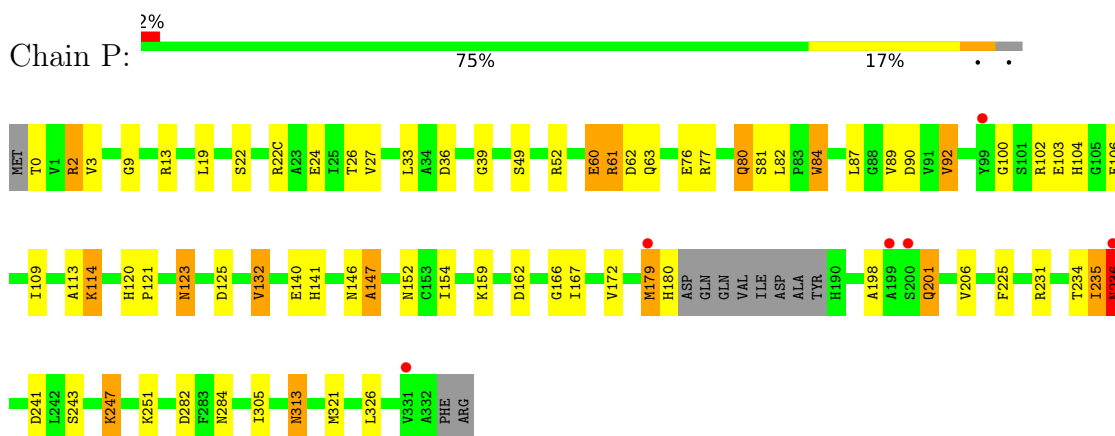
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

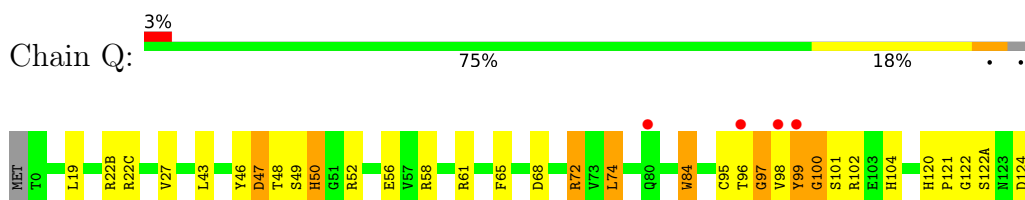
• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE

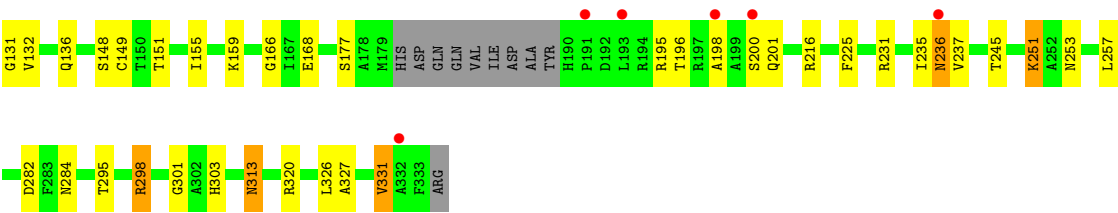


• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE

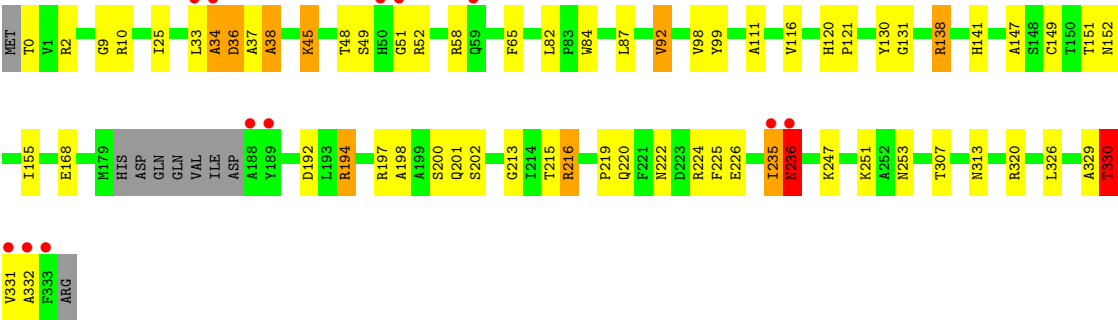
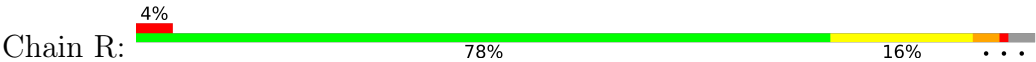


• Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE





● Molecule 1: D-ERYTHROSE-4-PHOSPHATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.206 , 0.266 0.201 , 0.256	Depositor DCC
R_{free} test set	2958 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10801	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.90	2/2543 (0.1%)	1.01	9/3457 (0.3%)
1	P	0.86	1/2572 (0.0%)	0.98	4/3498 (0.1%)
1	Q	0.83	0/2694	0.96	3/3665 (0.1%)
1	R	0.89	3/2619 (0.1%)	1.03	7/3561 (0.2%)
All	All	0.87	6/10428 (0.1%)	1.00	23/14181 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	237	VAL	C-O	-7.74	1.16	1.24
1	R	147	ALA	C-O	-7.06	1.17	1.24
1	P	236	ASN	C-O	-5.38	1.17	1.24
1	R	329	ALA	CA-CB	-5.26	1.45	1.53
1	R	45	LYS	C-O	-5.15	1.18	1.24
1	O	178	ALA	CA-CB	-5.12	1.44	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	235	ILE	N-CA-C	7.77	119.10	107.75
1	O	236	ASN	CB-CA-C	-7.32	100.78	111.91
1	P	236	ASN	N-CA-C	6.69	125.05	110.80
1	P	61	ARG	CB-CA-C	-6.49	108.41	117.23
1	O	193	LEU	N-CA-C	6.22	118.06	111.28
1	R	45	LYS	N-CA-C	6.18	118.10	111.36
1	R	332	ALA	N-CA-C	6.14	119.50	109.06
1	O	177	SER	CB-CA-C	-6.07	101.44	113.45
1	O	133	ASN	N-CA-C	5.86	119.56	111.71
1	Q	61	ARG	CB-CA-C	-5.80	109.87	116.54
1	R	236	ASN	N-CA-C	5.75	121.55	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	202	SER	N-CA-C	5.69	118.34	109.52
1	O	61	ARG	CB-CA-C	-5.66	110.06	116.63
1	O	236	ASN	N-CA-C	5.48	119.19	110.70
1	Q	301	GLY	N-CA-C	-5.45	100.84	110.86
1	P	92	VAL	CB-CA-C	-5.38	103.61	110.98
1	Q	131	GLY	N-CA-C	-5.36	108.31	114.69
1	R	38	ALA	N-CA-C	-5.32	105.48	111.28
1	P	132	VAL	N-CA-C	5.21	116.12	111.90
1	R	131	GLY	N-CA-C	-5.21	108.49	114.69
1	O	36	ASP	N-CA-C	5.12	117.72	110.50
1	O	317	PHE	N-CA-C	5.11	116.85	111.28
1	O	16	VAL	N-CA-C	5.02	115.24	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2499	0	2496	51	0
1	P	2526	0	2517	65	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	5	0
3	R	148	0	0	7	0
All	All	10801	0	10185	243	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 12.

All (243) 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: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:O:206:VAL:HG11	1:O:231:ARG:HD3	1.12	1.11
1:Q:96[B]:THR:CG2	1:Q:98[B]:VAL:CG2	2.26	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:HG13	1:R:331:VAL:O	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:HH11	1:Q:22(B)[B]:ARG:CG	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:CZ	1:P:61:ARG:HB2	2.11	0.81
1:Q:132:VAL:HG13	1:Q:159:LYS:HD3	1.61	0.80
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:36:ASP:OD2	1:R:36:ASP:C	2.30	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:R:330:THR:HG22	1:R:331:VAL:N	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:97[A]:GLY:O	1:Q:98[A]:VAL:C	2.34	0.71
1:R:48:THR:O	1:R:49:SER:HB3	1.91	0.70
1:Q:99[A]:TYR:H	1:Q:99[A]:TYR:HD2	1.39	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:Q:96[B]:THR:C	1:Q:98[B]:VAL:HG22	2.15	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:O:197:ARG:HH22	1:P:282:ASP:CG	2.01	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:P:201:GLN:HG2	3:Q:2019:HOH:O	1.96	0.66
1:Q:236[B]:ASN:ND2	1:Q:284:ASN:OD1	2.23	0.66
1:R:48:THR:CG2	3:R:2011:HOH:O	2.43	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: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:36:ASP:OD2	1:R:38:ALA:N	2.29	0.65
1:R:330:THR:HG22	1:R:331:VAL:H	1.62	0.65
1:O:17:ARG:O	1:O:21:GLU:HG3	1.97	0.64
1:Q:282:ASP:OD1	1:R:197:ARG:NH2	2.28	0.64
1:P:313:ASN:H	1:P:313:ASN:HD22	1.44	0.64
1:Q:282:ASP:CG	1:R:197:ARG:HH22	2.05	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:Q:96[B]:THR:C	1:Q:98[B]:VAL:N	2.56	0.63
1:P:201:GLN:CG	1:Q:48[A]:THR:HG21	2.28	0.63
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:P:49:SER:HB3	1:P:236:ASN:ND2	2.14	0.62
1:R:33:LEU:O	1:R:34:ALA:HB3	2.00	0.62
1:P:201:GLN:CD	1:Q:48[A]:THR:HG21	2.25	0.62
1:P:235:ILE:HD12	3:P:2096:HOH:O	1.98	0.62
1:P:313:ASN:H	1:P:313:ASN:ND2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:96[B]:THR:HG22	1:Q:96[B]:THR:O	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:HG3	1:Q:22(C):ARG:O	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:P:125:ASP:HB3	1:P:141:HIS:CD2	2.37	0.59
1:Q:96[B]:THR:CB	1:Q:98[B]:VAL:CG2	2.81	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: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:P:201:GLN:OE1	1:Q:48[A]:THR:HG21	2.04	0.57
1:Q:97[A]:GLY:CA	1:Q:120[A]:HIS:CE1	2.73	0.57
1:R:220:GLN:O	1:R:224:ARG:NH2	2.32	0.57
1:R:48:THR:O	1:R:49:SER:CB	2.53	0.57
1:O:60:GLU:HB3	1:O:65:PHE:HE1	1.70	0.56
1:P:235:ILE:CD1	3:P:2096:HOH:O	2.51	0.56
1:Q:96[B]:THR:C	1:Q:98[B]:VAL:H	2.13	0.56
1:P:236:ASN:OD1	1:P:236:ASN:N	2.38	0.56
1:Q:46[B]:TYR:CE1	1:Q:52[B]:ARG:NE	2.72	0.56
1:Q:96[B]:THR:HG21	1:Q:98[B]:VAL:CG2	2.32	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:O:258:LEU:HD22	3:O:2108:HOH:O	2.06	0.55
1:R:48:THR:HG21	3:R:2011:HOH:O	2.06	0.55
1:O:48:THR:HG21	1:R:198:ALA:HB3	1.87	0.55
1:P:36:ASP:OD1	1:P:36:ASP:C	2.48	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:HH11	1:R:194:ARG:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:48[A]:THR:CG2	3:Q:2019:HOH:O	2.55	0.54
1:Q:99[A]:TYR:CD2	1:Q:99[A]:TYR:N	2.73	0.53
1:Q:22(B)[B]:ARG:CG	1:Q:22(B)[B]:ARG:NH1	2.52	0.53
1:P:9:GLY:O	1:P:13:ARG:HG3	2.10	0.52
1:R:251:LYS:HE2	1:R:253:ASN:OD1	2.09	0.52
1:O:22(B):ARG:NH1	1:O:323:ASP:OD1	2.43	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:192:ASP:OD2	1:R:192:ASP:C	2.54	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:22(C):ARG:O	1:P:22(C):ARG:NE	2.45	0.50
1:P:36:ASP:OD1	1:P:36:ASP:O	2.30	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:R:9:GLY:O	1:R:10:ARG:C	2.54	0.49
1:Q:46[B]:TYR:OH	1:Q:52[B]:ARG:NH2	2.44	0.49
1:O:22(C):ARG:NH2	1:O:26:THR:HB	2.27	0.49
1:Q:99[B]:TYR:O	1:Q:120[B]:HIS:CD2	2.66	0.49
1:O:151:THR:HG22	1:O:155:ILE:HD12	1.95	0.48
1:P:114:LYS:H	1:P:114:LYS:CD	2.26	0.48
1:R:98:VAL:HG23	1:R:99:TYR:N	2.29	0.48
1:Q:49[B]:SER:O	1:Q:50[B]:HIS:CB	2.62	0.48
1:O:173:THR:OG1	1:P:241:ASP:OD1	2.25	0.47
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:HA	1:Q:84:TRP:CE3	2.49	0.47
1:Q:101[B]:SER:OG	1:Q:104:HIS:ND1	2.48	0.47
1:P:201:GLN:HG3	1:Q:48[A]:THR:HG23	1.92	0.47
1:P:102:ARG:O	1:P:106:GLU:HG2	2.16	0.46
1:P:146:ASN:O	1:P:147:ALA:CB	2.53	0.46
1:R:149:CYS:HB3	1:R:313:ASN:HB2	1.96	0.46
1:O:31:ASN:HB2	1:O:74:LEU:HD12	1.97	0.46
1:P:61:ARG:HH22	1:P:63:GLN:HG3	1.81	0.46
1:P:206:VAL:HG11	1:P:231:ARG:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:92:VAL:HG13	1:R:116:VAL:HG13	1.96	0.46
1:R:138:ARG:H	1:R:141:HIS:CE1	2.33	0.46
1:R:213:GLY:O	1:R:216[B]:ARG:HG3	2.15	0.46
1:O:10:ARG:HH11	1:O:10:ARG:HB3	1.80	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:P:2:ARG:NH1	1:P:87:LEU:O	2.46	0.46
1:Q:46[B]:TYR:CD1	1:Q:52[B]:ARG:HG2	2.51	0.46
1:Q:84:TRP:HA	1:Q:84:TRP:HE3	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:Q:72:ARG:NH1	3:Q:2044:HOH:O	2.33	0.45
1:R:84:TRP:HE3	1:R:84:TRP:HA	1.82	0.45
1:P:243:SER:HA	1:P:305:ILE:O	2.16	0.45
1:Q:327:ALA:O	1:Q:331:VAL:CG2	2.64	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:O:120:HIS:HB2	1:O:121:PRO:HD2	1.97	0.45
1:R:84:TRP:HA	1:R:84:TRP:CE3	2.52	0.45
1:O:103:GLU:CD	1:O:103:GLU:H	2.24	0.45
1:O:135:ASP:OD1	1:O:135:ASP:N	2.40	0.44
1:P:61:ARG:CB	1:P:61:ARG:NH1	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
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:122(A):SER:C	1:Q:216:ARG:HH12	2.27	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:P:321:MET:HE3	1:P:321:MET:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:GLU:HG2	1:P:104:HIS:H	1.84	0.42
1:P:154:ILE:HD12	1:P:154:ILE:HA	1.80	0.42
1:O:123:ASN:O	1:O:123:ASN:CG	2.63	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:216[A]:ARG:CG	3:R:2094:HOH:O	2.68	0.42
1:R:48:THR:O	1:R:48:THR:HG22	2.20	0.42
1:O:236:ASN:CG	1:O:236:ASN:O	2.57	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: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
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
2:R:1600:PO4:O4	3:R:2146:HOH:O	2.22	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:Q:96[B]:THR:HG21	1:Q:98[B]:VAL:HG21	1.97	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:NZ	1:P:247:LYS:HB3	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:O:93:LEU:HD23	1:O:321:MET:HG2	2.03	0.41
1:Q:46[B]:TYR:CE1	1:Q:52[B]:ARG:HG2	2.55	0.41
1:R:120:HIS:HB2	1:R:121:PRO:CD	2.50	0.41
1:P:19:LEU:HD22	1:P:27:VAL:HG23	2.03	0.40
1:Q:95:CYS:C	1:Q:97[B]:GLY:H	2.29	0.40
1:P:80:GLN:H	1:P:80:GLN:HG3	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%)	36	46
1	P	324/339 (96%)	305 (94%)	15 (5%)	4 (1%)	10	12
1	Q	340/339 (100%)	304 (89%)	24 (7%)	12 (4%)	3	1
1	R	329/339 (97%)	312 (95%)	15 (5%)	2 (1%)	21	27
All	All	1313/1356 (97%)	1228 (94%)	66 (5%)	19 (1%)	11	9

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
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%)	250 (94%)	17 (6%)	16	23
1	P	269/280 (96%)	243 (90%)	26 (10%)	8	10
1	Q	280/280 (100%)	261 (93%)	19 (7%)	14	20
1	R	273/280 (98%)	258 (94%)	15 (6%)	19	28
All	All	1089/1120 (97%)	1012 (93%)	77 (7%)	14	19

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	10	ARG
1	O	24	GLU
1	O	36	ASP
1	O	49	SER
1	O	58	ARG
1	O	64	LEU
1	O	74	LEU
1	O	78	SER
1	O	80	GLN
1	O	103	GLU
1	O	135	ASP
1	O	177	SER
1	O	179	MET
1	O	225	PHE
1	O	250	VAL
1	O	257	LEU
1	O	258	LEU
1	P	0	THR
1	P	2	ARG
1	P	3	VAL
1	P	24	GLU
1	P	26	THR
1	P	52	ARG
1	P	60	GLU

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Mol	Chain	Res	Type
1	P	77	ARG
1	P	80	GLN
1	P	84	TRP
1	P	92	VAL
1	P	114	LYS
1	P	123	ASN
1	P	132	VAL
1	P	140	GLU
1	P	152	ASN
1	P	159	LYS
1	P	172	VAL
1	P	179	MET
1	P	201	GLN
1	P	225	PHE
1	P	235	ILE
1	P	247	LYS
1	P	251	LYS
1	P	313	ASN
1	P	326	LEU
1	Q	56	GLU
1	Q	72	ARG
1	Q	74	LEU
1	Q	84	TRP
1	Q	99[A]	TYR
1	Q	99[B]	TYR
1	Q	136	GLN
1	Q	168	GLU
1	Q	195	ARG
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	298	ARG
1	Q	313	ASN
1	Q	326	LEU
1	Q	331	VAL
1	R	0	THR
1	R	36	ASP
1	R	45	LYS
1	R	52	ARG

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Mol	Chain	Res	Type
1	R	92	VAL
1	R	138	ARG
1	R	152	ASN
1	R	194	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	176	HIS
1	O	260	GLN
1	O	264	GLN
1	O	296	GLN
1	P	59	GLN
1	P	260	GLN
1	P	264	GLN
1	P	296	GLN
1	P	313	ASN
1	Q	176	HIS
1	Q	313	ASN
1	R	14	ASN
1	R	50	HIS
1	R	59	GLN
1	R	176	HIS
1	R	236	ASN
1	R	264	GLN
1	R	313	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	Q	1600	-	4,4,4	0.95	0	6,6,6	0.80	0
2	PO4	P	1600	-	4,4,4	0.89	0	6,6,6	0.51	0
2	PO4	R	1600	-	4,4,4	1.04	0	6,6,6	1.11	0
2	PO4	O	1600	-	4,4,4	0.93	0	6,6,6	0.68	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	1600	PO4	1	0

5.7 Other polymers [i](#)

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	324/339 (95%)	0.04	7 (2%) 62 64	17, 34, 52, 60	0
1	P	328/339 (96%)	0.10	6 (1%) 67 69	18, 34, 57, 68	0
1	Q	328/339 (96%)	-0.08	10 (3%) 52 54	13, 27, 49, 78	16 (4%)
1	R	330/339 (97%)	0.05	12 (3%) 46 48	11, 31, 50, 64	3 (0%)
All	All	1310/1356 (96%)	0.03	35 (2%) 56 58	11, 31, 53, 78	19 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	236[A]	ASN	3.7
1	P	331	VAL	3.4
1	R	331	VAL	3.2
1	Q	99[A]	TYR	3.1
1	P	179	MET	3.1
1	P	236	ASN	3.0
1	R	59	GLN	2.9
1	Q	98[A]	VAL	2.9
1	O	98	VAL	2.8
1	R	34	ALA	2.7
1	P	200	SER	2.6
1	O	331	VAL	2.6
1	O	99	TYR	2.6
1	O	192	ASP	2.5
1	Q	198	ALA	2.5
1	R	333	PHE	2.4
1	P	199	ALA	2.4
1	Q	191	PRO	2.4
1	Q	200	SER	2.4
1	R	50	HIS	2.3
1	R	236	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	193	LEU	2.3
1	O	179	MET	2.3
1	Q	96[A]	THR	2.1
1	R	332	ALA	2.1
1	P	99	TYR	2.1
1	R	189	TYR	2.1
1	Q	332	ALA	2.1
1	O	193	LEU	2.1
1	Q	80	GLN	2.1
1	R	51	GLY	2.1
1	R	33	LEU	2.0
1	R	188	ALA	2.0
1	O	50	HIS	2.0
1	R	235	ILE	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 oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	O	1600	5/5	0.84	0.11	45,45,47,48	5
2	PO4	R	1600	5/5	0.93	0.09	33,34,35,35	5
2	PO4	Q	1600	5/5	0.94	0.09	40,40,41,44	5
2	PO4	P	1600	5/5	0.94	0.07	33,33,34,36	5

6.5 Other polymers [i](#)

There are no such residues in this entry.