



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:33 AM BST

PDB ID : 4LRE  
Title : Phosphopentomutase soaked with 2,3-dideoxyribose 5-phosphate  
Authors : Birmingham, W.A.; Starbird, C.A.; Panosian, T.D.; Nannemann, D.P.; Iversen, T.M.; Bachmann, B.O.  
Deposited on : 2013-07-19  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

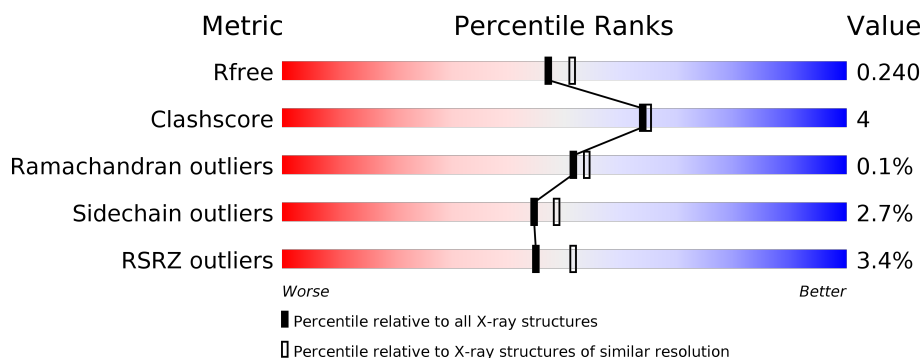
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	A	416	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	416	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
1	C	416	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9898 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 Phosphopentomutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	P	S	14	0	0
			3068	1939	505	606	1	17			
1	B	391	Total	C	N	O	P	S	7	0	0
			3068	1939	505	606	1	17			
1	C	390	Total	C	N	O	P	S	47	0	0
			3060	1935	503	604	1	17			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q818Z9
A	-20	GLY	-	expression tag	UNP Q818Z9
A	-19	SER	-	expression tag	UNP Q818Z9
A	-18	SER	-	expression tag	UNP Q818Z9
A	-17	HIS	-	expression tag	UNP Q818Z9
A	-16	HIS	-	expression tag	UNP Q818Z9
A	-15	HIS	-	expression tag	UNP Q818Z9
A	-14	HIS	-	expression tag	UNP Q818Z9
A	-13	HIS	-	expression tag	UNP Q818Z9
A	-12	HIS	-	expression tag	UNP Q818Z9
A	-11	SER	-	expression tag	UNP Q818Z9
A	-10	SER	-	expression tag	UNP Q818Z9
A	-9	GLY	-	expression tag	UNP Q818Z9
A	-8	LEU	-	expression tag	UNP Q818Z9
A	-7	VAL	-	expression tag	UNP Q818Z9
A	-6	PRO	-	expression tag	UNP Q818Z9
A	-5	ARG	-	expression tag	UNP Q818Z9
A	-4	GLY	-	expression tag	UNP Q818Z9
A	-3	SER	-	expression tag	UNP Q818Z9
A	-2	HIS	-	expression tag	UNP Q818Z9
A	-1	MET	-	expression tag	UNP Q818Z9
A	0	ALA	-	expression tag	UNP Q818Z9
A	1	SER	-	expression tag	UNP Q818Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	expression tag	UNP Q818Z9
B	-20	GLY	-	expression tag	UNP Q818Z9
B	-19	SER	-	expression tag	UNP Q818Z9
B	-18	SER	-	expression tag	UNP Q818Z9
B	-17	HIS	-	expression tag	UNP Q818Z9
B	-16	HIS	-	expression tag	UNP Q818Z9
B	-15	HIS	-	expression tag	UNP Q818Z9
B	-14	HIS	-	expression tag	UNP Q818Z9
B	-13	HIS	-	expression tag	UNP Q818Z9
B	-12	HIS	-	expression tag	UNP Q818Z9
B	-11	SER	-	expression tag	UNP Q818Z9
B	-10	SER	-	expression tag	UNP Q818Z9
B	-9	GLY	-	expression tag	UNP Q818Z9
B	-8	LEU	-	expression tag	UNP Q818Z9
B	-7	VAL	-	expression tag	UNP Q818Z9
B	-6	PRO	-	expression tag	UNP Q818Z9
B	-5	ARG	-	expression tag	UNP Q818Z9
B	-4	GLY	-	expression tag	UNP Q818Z9
B	-3	SER	-	expression tag	UNP Q818Z9
B	-2	HIS	-	expression tag	UNP Q818Z9
B	-1	MET	-	expression tag	UNP Q818Z9
B	0	ALA	-	expression tag	UNP Q818Z9
B	1	SER	-	expression tag	UNP Q818Z9
C	-21	MET	-	expression tag	UNP Q818Z9
C	-20	GLY	-	expression tag	UNP Q818Z9
C	-19	SER	-	expression tag	UNP Q818Z9
C	-18	SER	-	expression tag	UNP Q818Z9
C	-17	HIS	-	expression tag	UNP Q818Z9
C	-16	HIS	-	expression tag	UNP Q818Z9
C	-15	HIS	-	expression tag	UNP Q818Z9
C	-14	HIS	-	expression tag	UNP Q818Z9
C	-13	HIS	-	expression tag	UNP Q818Z9
C	-12	HIS	-	expression tag	UNP Q818Z9
C	-11	SER	-	expression tag	UNP Q818Z9
C	-10	SER	-	expression tag	UNP Q818Z9
C	-9	GLY	-	expression tag	UNP Q818Z9
C	-8	LEU	-	expression tag	UNP Q818Z9
C	-7	VAL	-	expression tag	UNP Q818Z9
C	-6	PRO	-	expression tag	UNP Q818Z9
C	-5	ARG	-	expression tag	UNP Q818Z9
C	-4	GLY	-	expression tag	UNP Q818Z9
C	-3	SER	-	expression tag	UNP Q818Z9

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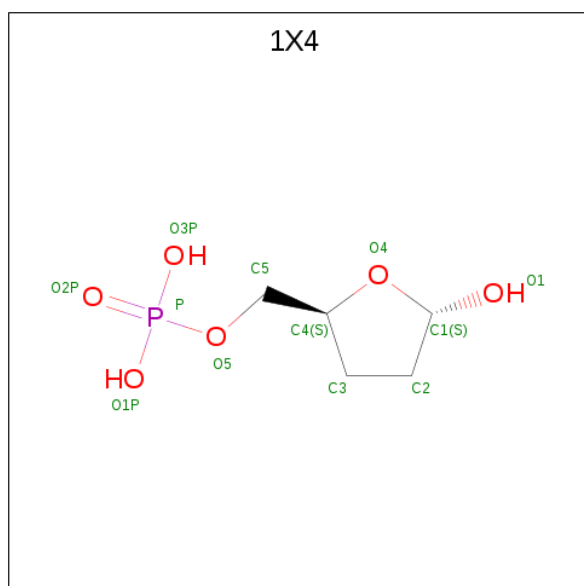
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q818Z9
C	-1	MET	-	expression tag	UNP Q818Z9
C	0	ALA	-	expression tag	UNP Q818Z9
C	1	SER	-	expression tag	UNP Q818Z9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Mn 4 4	0	0
2	A	3	Total Mn 3 3	0	0
2	C	3	Total Mn 3 3	0	0

- Molecule 3 is 2,3-dideoxy-5-O-phosphono-alpha-D-ribofuranose (three-letter code: 1X4) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 12 5 6 1	0	0

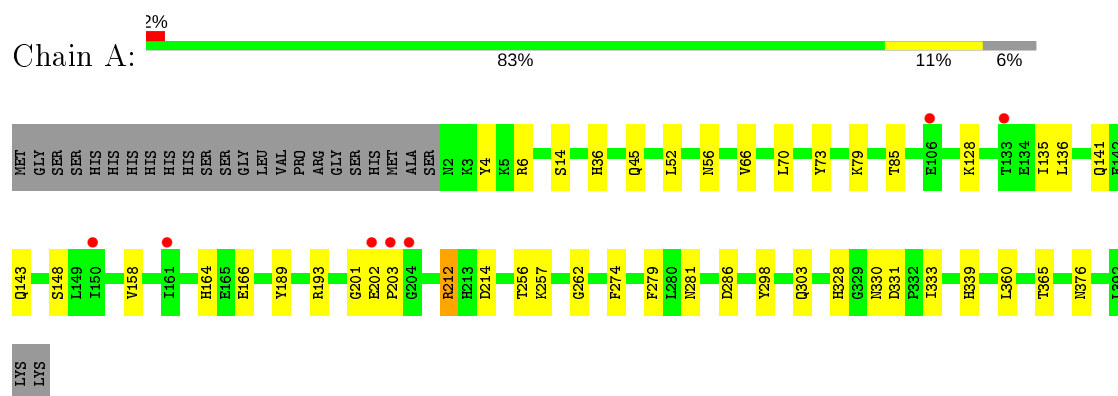
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total 246	O 246	0	0
4	B	294	Total 294	O 294	0	0
4	C	140	Total 140	O 140	0	0

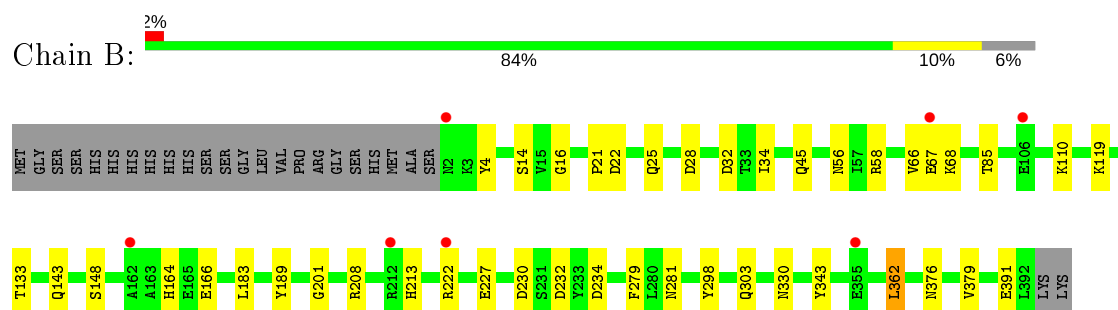
### 3 Residue-property plots [i](#)

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.

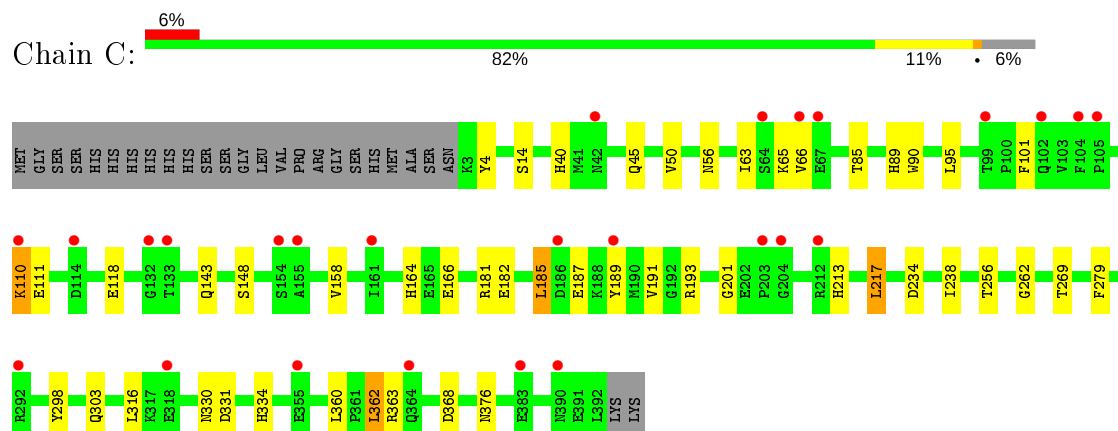
#### • Molecule 1: Phosphopentomutase



#### • Molecule 1: Phosphopentomutase



#### • Molecule 1: Phosphopentomutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.50 Å   76.52 Å   107.29 Å 90.00°   108.76°   90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.10) 96.5 (19.99-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.09 Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, $R_{free}$	0.193   ,   0.239 0.194   ,   0.240	Depositor DCC
$R_{free}$ test set	3900 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.7	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	0.94	EDS
Total number of atoms	9898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: TPO, MN, 1X4

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	A	0.48	1/3117 (0.0%)	0.60	0/4208
1	B	0.48	0/3117	0.63	1/4208 (0.0%)
1	C	0.70	3/3109 (0.1%)	0.72	8/4197 (0.2%)
All	All	0.56	4/9343 (0.0%)	0.65	9/12613 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	GLU	CB-CG	19.64	1.89	1.52
1	C	187	GLU	CA-CB	-15.69	1.19	1.53
1	C	110	LYS	CB-CG	11.50	1.83	1.52
1	A	257	LYS	CB-CG	-8.28	1.30	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	GLU	CB-CA-C	-11.32	87.75	110.40
1	C	187	GLU	N-CA-CB	10.48	129.46	110.60
1	C	110	LYS	CA-CB-CG	-8.85	93.94	113.40
1	C	111	GLU	CB-CG-CD	-7.97	92.68	114.20
1	C	187	GLU	CA-CB-CG	-6.68	98.69	113.40
1	C	182	GLU	CG-CD-OE1	-6.16	105.98	118.30
1	C	182	GLU	CG-CD-OE2	6.11	130.51	118.30
1	B	362	LEU	CA-CB-CG	5.68	128.37	115.30
1	C	362	LEU	CA-CB-CG	5.55	128.07	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3068	0	3007	30	0
1	B	3068	0	3007	25	0
1	C	3060	0	3001	25	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
3	A	12	0	2	0	0
4	A	246	0	0	2	0
4	B	294	0	0	3	0
4	C	140	0	0	1	0
All	All	9898	0	9017	76	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 4.

All (76) 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:B:4:TYR:H	1:B:376:ASN:HD21	1.10	0.99
1:A:4:TYR:H	1:A:376:ASN:HD21	1.07	0.93
1:A:164:HIS:HD2	1:A:166:GLU:H	1.16	0.93
1:C:4:TYR:H	1:C:376:ASN:HD21	1.17	0.92
1:B:164:HIS:HD2	1:B:166:GLU:H	1.27	0.81
1:C:164:HIS:HD2	1:C:166:GLU:H	1.33	0.74
1:B:227:GLU:OE2	4:B:767:HOH:O	2.07	0.72
1:A:164:HIS:CD2	1:A:166:GLU:H	2.08	0.64
1:B:45:GLN:H	1:B:303:GLN:HE21	1.45	0.63
1:A:45:GLN:H	1:A:303:GLN:HE21	1.46	0.63
1:B:56:ASN:HD21	1:B:66:VAL:H	1.46	0.62
1:A:4:TYR:N	1:A:376:ASN:HD21	1.88	0.62
1:B:164:HIS:CD2	1:B:166:GLU:H	2.15	0.62
1:B:28:ASP:OD1	4:B:736:HOH:O	2.16	0.61
1:B:227:GLU:HG3	1:B:379:VAL:HB	1.83	0.60
1:A:36:HIS:HD2	1:A:331:ASP:OD2	1.86	0.58
1:B:232:ASP:OD1	1:C:213:HIS:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HB2	1:A:203:PRO:HD2	1.85	0.57
1:A:56:ASN:HD21	1:A:66:VAL:H	1.53	0.57
1:C:101:PHE:HE2	1:C:217:LEU:HD23	1.69	0.57
1:C:14:SER:HB2	1:C:330:ASN:HB2	1.86	0.57
1:A:202:GLU:HB2	1:A:203:PRO:CD	2.35	0.56
1:A:85:TPO:O1P	1:A:339:HIS:HE1	1.89	0.56
1:C:164:HIS:HE1	1:C:201:GLY:O	1.88	0.56
1:A:14:SER:HB2	1:A:330:ASN:HB2	1.88	0.56
1:B:164:HIS:HE1	1:B:201:GLY:O	1.88	0.56
1:B:213:HIS:HD2	1:C:234:ASP:OD1	1.88	0.56
1:A:85:TPO:O1P	1:A:339:HIS:CE1	2.59	0.55
1:B:4:TYR:H	1:B:376:ASN:ND2	1.93	0.54
1:A:333:ILE:HG22	1:A:333:ILE:O	2.07	0.54
1:A:36:HIS:CD2	1:A:331:ASP:OD2	2.61	0.53
1:C:56:ASN:HD21	1:C:66:VAL:H	1.55	0.53
1:C:40:HIS:HB2	4:C:512:HOH:O	2.09	0.53
1:C:158:VAL:HG12	1:C:193:ARG:HB3	1.91	0.52
1:A:164:HIS:HE1	1:A:201:GLY:O	1.93	0.51
1:B:119:LYS:HE3	1:B:183:LEU:HD21	1.92	0.51
1:A:212:ARG:HD3	1:A:214:ASP:OD1	2.10	0.51
1:A:158:VAL:HG12	1:A:193:ARG:HB3	1.92	0.50
1:A:256:THR:HG21	1:A:262:GLY:HA2	1.94	0.50
1:C:143:GLN:HG2	1:C:148:SER:O	2.12	0.49
1:A:45:GLN:H	1:A:303:GLN:NE2	2.10	0.49
1:B:222:ARG:NH2	1:B:230:ASP:OD1	2.38	0.48
1:B:14:SER:HB2	1:B:330:ASN:HB2	1.93	0.48
1:C:85:TPO:O	1:C:89:HIS:HD2	1.97	0.47
1:C:256:THR:HG21	1:C:262:GLY:HA2	1.96	0.47
1:B:143:GLN:HG2	1:B:148:SER:O	2.15	0.47
1:C:45:GLN:H	1:C:303:GLN:HE21	1.64	0.46
1:B:21:PRO:HD3	1:B:343:TYR:CZ	2.51	0.46
1:A:143:GLN:HG2	1:A:148:SER:O	2.15	0.46
1:A:141:GLN:HG3	1:A:203:PRO:HG3	1.99	0.45
1:B:22:ASP:O	1:B:25:GLN:HG2	2.17	0.45
1:A:6:ARG:HD2	1:A:274:PHE:CE1	2.51	0.45
1:C:331:ASP:HB3	1:C:334:HIS:HB2	1.99	0.45
1:A:14:SER:HB2	1:A:330:ASN:CB	2.48	0.44
1:B:234:ASP:OD1	1:C:213:HIS:HD2	2.01	0.43
1:C:363:ARG:NE	1:C:368:ASP:OD1	2.51	0.43
1:A:128:LYS:HE2	4:A:746:HOH:O	2.18	0.43
1:A:36:HIS:HB3	1:A:333:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ASN:HD21	1:C:66:VAL:HG22	1.84	0.42
1:B:32:ASP:OD2	1:B:58:ARG:NH2	2.42	0.42
1:B:133:THR:OG1	1:B:208:ARG:NH1	2.52	0.42
1:C:14:SER:HB2	1:C:330:ASN:CB	2.47	0.42
1:B:16:GLY:O	1:B:34:ILE:HG13	2.18	0.42
1:B:68:LYS:HE2	4:B:688:HOH:O	2.20	0.42
1:A:56:ASN:HB3	1:A:73:TYR:CE2	2.55	0.42
1:C:45:GLN:H	1:C:303:GLN:NE2	2.17	0.42
1:B:232:ASP:OD1	1:C:213:HIS:CE1	2.71	0.41
1:C:90:TRP:HB3	1:C:95:LEU:HD12	2.02	0.41
1:C:50:VAL:HG22	1:C:63:ILE:HG23	2.01	0.41
1:C:238:ILE:HD11	1:C:269:THR:HG21	2.02	0.41
1:A:85:TPO:O2P	1:A:286:ASP:OD1	2.38	0.41
1:C:181:ARG:O	1:C:185:LEU:HD13	2.21	0.41
1:B:56:ASN:HD22	1:B:56:ASN:H	1.69	0.41
1:A:52:LEU:HA	1:A:70:LEU:HB2	2.03	0.41
1:A:202:GLU:HB3	4:A:651:HOH:O	2.21	0.40
1:A:79:LYS:HD2	1:A:365:THR:HB	2.02	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	A	388/416 (93%)	374 (96%)	13 (3%)	1 (0%)	41	41
1	B	388/416 (93%)	375 (97%)	13 (3%)	0	100	100
1	C	387/416 (93%)	369 (95%)	18 (5%)	0	100	100
All	All	1163/1248 (93%)	1118 (96%)	44 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	HIS

### 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	A	332/353 (94%)	324 (98%)	8 (2%)	49	53
1	B	332/353 (94%)	324 (98%)	8 (2%)	49	53
1	C	331/353 (94%)	320 (97%)	11 (3%)	38	40
All	All	995/1059 (94%)	968 (97%)	27 (3%)	44	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
1	A	136	LEU
1	A	189	TYR
1	A	212	ARG
1	A	279	PHE
1	A	281	ASN
1	A	298	TYR
1	A	360	LEU
1	B	67	GLU
1	B	110	LYS
1	B	189	TYR
1	B	279	PHE
1	B	281	ASN
1	B	298	TYR
1	B	362	LEU
1	B	391	GLU
1	C	65	LYS
1	C	110	LYS
1	C	185	LEU
1	C	189	TYR
1	C	191	VAL
1	C	217	LEU

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Mol	Chain	Res	Type
1	C	279	PHE
1	C	298	TYR
1	C	316	LEU
1	C	360	LEU
1	C	362	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	48	ASN
1	A	56	ASN
1	A	89	HIS
1	A	164	HIS
1	A	205	ASN
1	A	259	ASN
1	A	281	ASN
1	A	303	GLN
1	A	358	GLN
1	A	376	ASN
1	A	390	ASN
1	B	56	ASN
1	B	89	HIS
1	B	102	GLN
1	B	164	HIS
1	B	205	ASN
1	B	211	ASN
1	B	213	HIS
1	B	259	ASN
1	B	281	ASN
1	B	303	GLN
1	B	376	ASN
1	C	45	GLN
1	C	56	ASN
1	C	77	GLN
1	C	89	HIS
1	C	164	HIS
1	C	213	HIS
1	C	259	ASN
1	C	281	ASN
1	C	303	GLN
1	C	376	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPO	A	85	1,2	8,10,11	0.53	0	10,14,16	1.19	0
1	TPO	B	85	1,2	8,10,11	1.00	1 (12%)	10,14,16	0.86	0
1	TPO	C	85	1,2	8,10,11	0.86	0	10,14,16	0.88	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
1	TPO	A	85	1,2	-	1/9/11/13	-
1	TPO	B	85	1,2	-	3/9/11/13	-
1	TPO	C	85	1,2	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	TPO	P-OG1	2.18	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	85	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	85	TPO	CB-OG1-P-O1P
1	B	85	TPO	CB-OG1-P-O3P
1	A	85	TPO	O-C-CA-CB
1	C	85	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	85	TPO	3	0
1	C	85	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	1X4	A	404	-	12,12,12	1.39	1 (8%)	13,17,17	1.13	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1X4	A	404	-	-	3/6/15/15	0/1/1/1

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	1X4	P-O2P	3.75	1.62	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	404	1X4	O3P-P-O5	2.79	114.17	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	1X4	C5-O5-P-O1P
3	A	404	1X4	C5-O5-P-O2P
3	A	404	1X4	C5-O5-P-O3P

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 ⓘ

### 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	A	390/416 (93%)	-0.02	7 (1%)	68 72	15, 21, 31, 36	17 (4%)
1	B	390/416 (93%)	0.09	7 (1%)	68 72	15, 21, 30, 43	13 (3%)
1	C	389/416 (93%)	0.43	26 (6%)	17 22	18, 27, 39, 46	23 (5%)
All	All	1169/1248 (93%)	0.17	40 (3%)	45 51	15, 23, 35, 46	53 (4%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASN	4.9
1	C	355	GLU	4.7
1	C	105	PRO	4.4
1	B	222	ARG	4.1
1	C	204	GLY	3.9
1	C	189	TYR	3.5
1	C	42	ASN	3.3
1	C	318	GLU	3.2
1	C	64	SER	3.1
1	B	212	ARG	2.9
1	C	161	ILE	2.8
1	C	110	LYS	2.8
1	C	364	GLN	2.7
1	C	212	ARG	2.7
1	A	202	GLU	2.6
1	B	355	GLU	2.6
1	B	67	GLU	2.6
1	C	390	ASN	2.5
1	C	67	GLU	2.5
1	C	133	THR	2.5
1	C	114	ASP	2.4
1	C	104	PHE	2.3
1	C	154	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	66	VAL	2.3
1	C	383	GLU	2.2
1	C	99	THR	2.2
1	C	155	ALA	2.2
1	A	161	ILE	2.1
1	B	162	ALA	2.1
1	B	106	GLU	2.1
1	C	186	ASP	2.1
1	C	203	PRO	2.1
1	A	150	ILE	2.1
1	A	203	PRO	2.1
1	C	132	GLY	2.1
1	A	106	GLU	2.1
1	C	292	ARG	2.1
1	A	133	THR	2.0
1	A	204	GLY	2.0
1	C	102	GLN	2.0

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

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(Å <sup>2</sup> )	Q<0.9
1	TPO	C	85	11/12	0.94	0.16	25,26,28,28	4
1	TPO	B	85	11/12	0.96	0.16	20,22,24,24	4
1	TPO	A	85	11/12	0.96	0.16	18,19,20,20	4

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	1X4	A	404	12/12	0.79	0.26	35,35,36,36	12
2	MN	B	404	1/1	0.81	0.09	54,54,54,54	1
2	MN	B	403	1/1	0.94	0.10	49,49,49,49	1
2	MN	A	403	1/1	0.98	0.04	33,33,33,33	1
2	MN	C	403	1/1	0.98	0.05	46,46,46,46	0
2	MN	A	402	1/1	0.99	0.12	22,22,22,22	0
2	MN	C	401	1/1	0.99	0.10	29,29,29,29	0
2	MN	C	402	1/1	0.99	0.12	27,27,27,27	0
2	MN	B	402	1/1	1.00	0.13	22,22,22,22	0
2	MN	B	401	1/1	1.00	0.13	21,21,21,21	0
2	MN	A	401	1/1	1.00	0.12	19,19,19,19	0

## 6.5 Other polymers

There are no such residues in this entry.