



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 02:59 PM EDT

PDB ID : 2R87  
Title : Crystal structure of PurP from *Pyrococcus furiosus* complexed with ADP  
Authors : Zhang, Y.; White, R.H.; Ealick, S.E.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

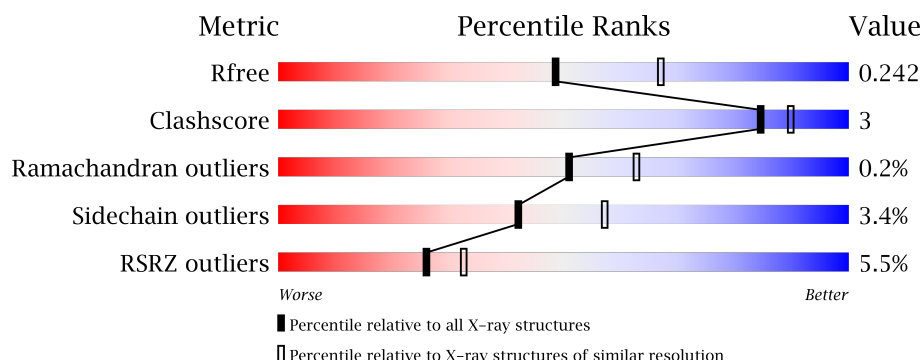
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	334	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
1	B	334	<div> <div>6%</div> <div>87%</div> <div>13%</div> </div>
1	C	334	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	D	334	<div> <div>8%</div> <div>87%</div> <div>13%</div> </div>
1	E	334	<div> <div>6%</div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	501	-	-	-	X

## 2 Entry composition [i](#)

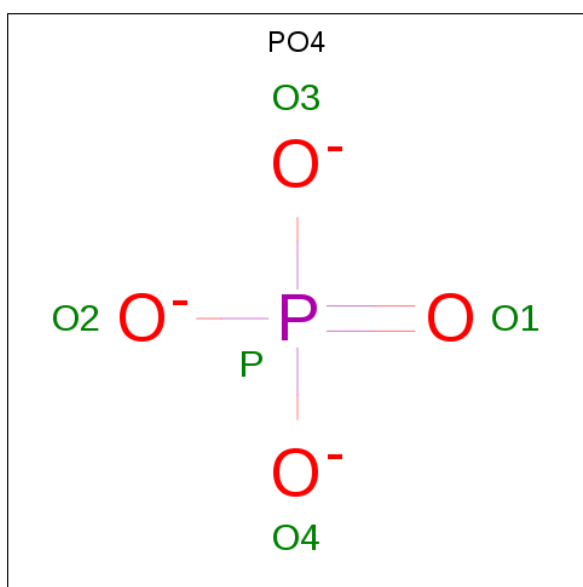
There are 4 unique types of molecules in this entry. The entry contains 17028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PurP protein PF1517.

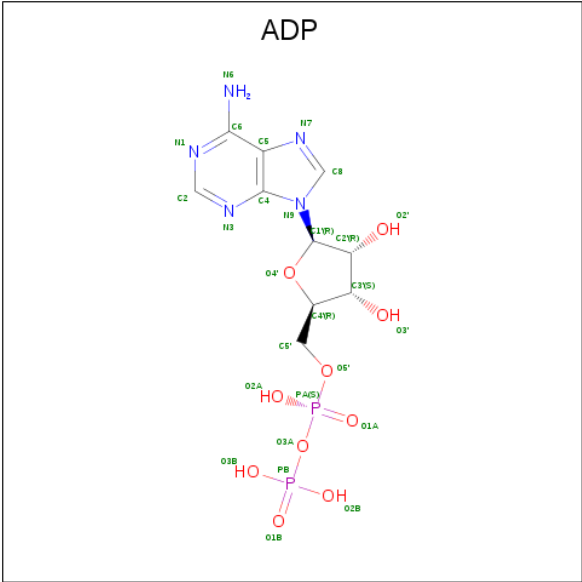
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2705	1752	448	496	9			
1	B	334	Total	C	N	O	S	0	0	0
			2705	1752	448	496	9			
1	C	334	Total	C	N	O	S	0	0	0
			2705	1752	448	496	9			
1	D	334	Total	C	N	O	S	0	0	0
			2705	1752	448	496	9			
1	E	334	Total	C	N	O	S	0	0	0
			2705	1752	448	496	9			
1	F	334	Total	C	N	O	S	0	0	0
			2705	1752	448	496	9			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

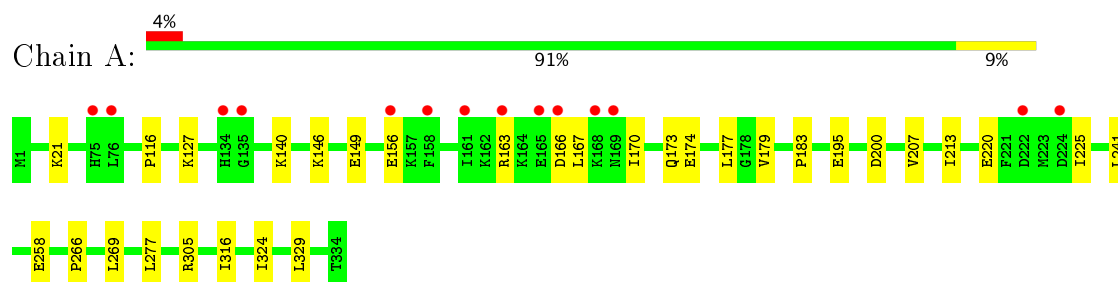
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	89	Total	O	0	0
			89	89		
4	C	95	Total	O	0	0
			95	95		
4	D	91	Total	O	0	0
			91	91		
4	E	83	Total	O	0	0
			83	83		
4	F	82	Total	O	0	0
			82	82		

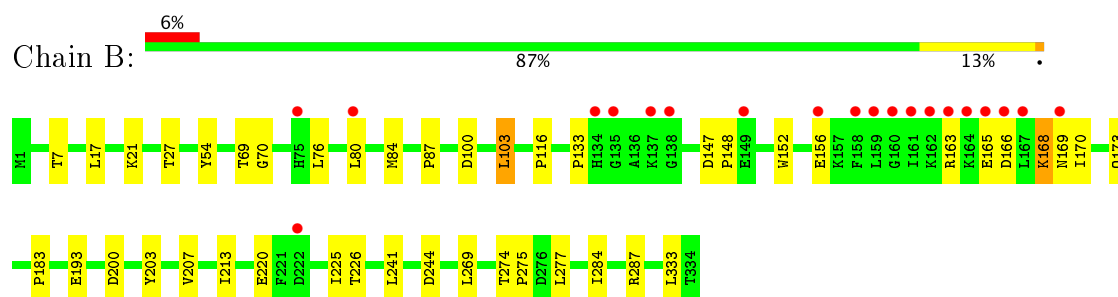
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

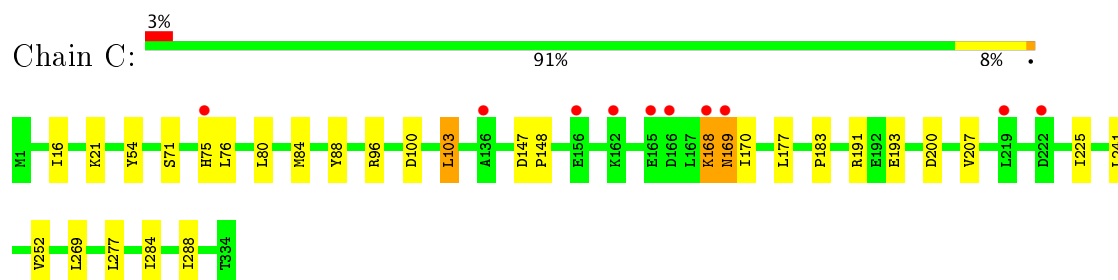
#### • Molecule 1: PurP protein PF1517



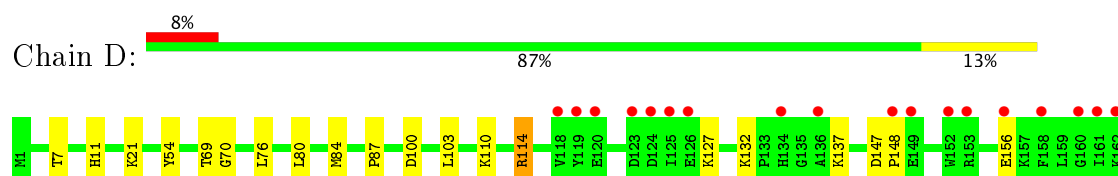
#### • Molecule 1: PurP protein PF1517



#### • Molecule 1: PurP protein PF1517

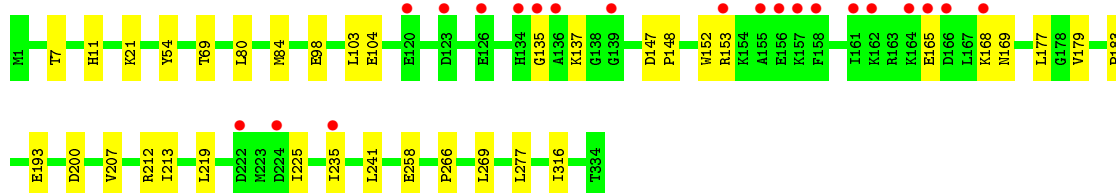
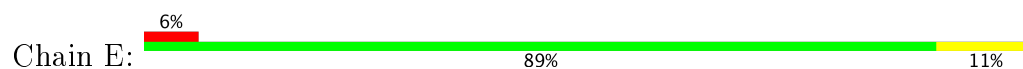


#### • Molecule 1: PurP protein PF1517

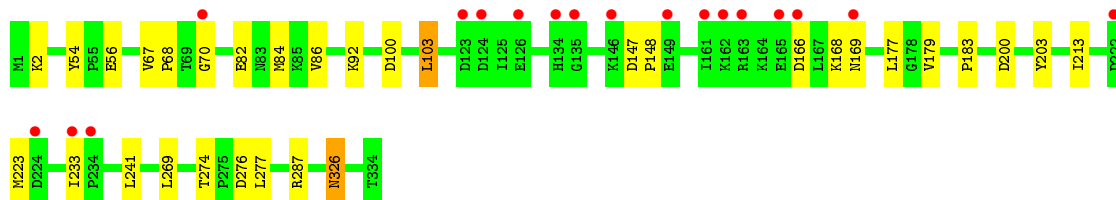
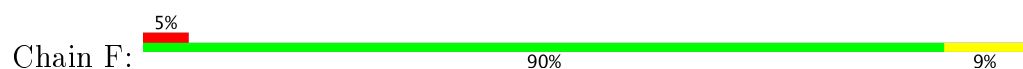




● Molecule 1: PurP protein PF1517



● Molecule 1: PurP protein PF1517





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.09Å 127.22Å 121.67Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	42.64 – 2.30 40.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.64-2.30) 98.7 (40.42-2.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, $R_{free}$	0.201 , 0.244 0.200 , 0.242	Depositor DCC
$R_{free}$ test set	4941 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: PO4, ADP

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	0.39	0/2768	0.53	0/3742
1	B	0.38	0/2768	0.52	0/3742
1	C	0.39	0/2768	0.53	0/3742
1	D	0.38	0/2768	0.52	0/3742
1	E	0.39	0/2768	0.52	0/3742
1	F	0.38	0/2768	0.51	0/3742
All	All	0.39	0/16608	0.52	0/22452

There are no bond length outliers.

There are no bond angle outliers.

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	A	2705	0	2727	13	0
1	B	2705	0	2727	21	0
1	C	2705	0	2727	14	0
1	D	2705	0	2727	20	0
1	E	2705	0	2727	16	0
1	F	2705	0	2727	17	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	0	0	0
2	C	20	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	1	0
2	F	15	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
4	A	101	0	0	0	0
4	B	89	0	0	0	0
4	C	95	0	0	0	0
4	D	91	0	0	0	0
4	E	83	0	0	0	0
4	F	82	0	0	0	0
All	All	17028	0	16434	90	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 3.

All (90) 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:A:146:LYS:HB2	1:B:220:GLU:HG3	1.47	0.97
1:D:70:GLY:HA2	1:D:287:ARG:HD2	1.60	0.84
1:D:213:ILE:HD11	1:F:177:LEU:HD13	1.75	0.68
1:F:147:ASP:HB2	1:F:148:PRO:HD2	1.78	0.66
1:F:70:GLY:HA2	1:F:287:ARG:HD2	1.78	0.65
1:A:127:LYS:HD2	1:A:174:GLU:HG3	1.79	0.63
1:E:147:ASP:HB2	1:E:148:PRO:HD2	1.81	0.62
1:F:241:LEU:HD21	1:F:277:LEU:HD22	1.83	0.61
1:C:147:ASP:HB2	1:C:148:PRO:HD2	1.83	0.60
1:F:274:THR:OG1	1:F:276:ASP:OD2	2.17	0.59
1:B:70:GLY:HA2	1:B:287:ARG:HD2	1.85	0.58
1:F:147:ASP:HB2	1:F:148:PRO:CD	2.34	0.57
1:E:147:ASP:HB2	1:E:148:PRO:CD	2.36	0.56
1:D:54:TYR:OH	1:D:84:MET:HB2	2.06	0.56
1:C:147:ASP:HB2	1:C:148:PRO:CD	2.36	0.55
1:B:100:ASP:HB3	1:B:103:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:VAL:HG23	1:D:225:ILE:HD11	1.88	0.55
1:A:183:PRO:HD2	1:A:269:LEU:O	2.07	0.54
1:C:54:TYR:HB2	1:C:76:LEU:HD21	1.88	0.54
1:A:213:ILE:HD11	1:C:177:LEU:HD13	1.89	0.54
1:C:252:VAL:HG11	1:C:284:ILE:HD12	1.89	0.53
1:A:195:GLU:OE2	1:A:305:ARG:NH1	2.42	0.53
1:D:147:ASP:HB2	1:D:148:PRO:HD2	1.92	0.52
1:D:177:LEU:HD13	1:E:213:ILE:HD11	1.91	0.52
1:B:241:LEU:HD21	1:B:277:LEU:HD22	1.92	0.52
1:E:177:LEU:HD13	1:F:213:ILE:HD11	1.91	0.51
1:D:132:LYS:HD2	1:D:171:GLN:HE21	1.76	0.51
1:D:110:LYS:HE2	1:D:258:GLU:HG3	1.92	0.51
1:E:183:PRO:HD2	1:E:269:LEU:O	2.11	0.51
1:D:147:ASP:HB2	1:D:148:PRO:CD	2.41	0.50
1:B:76:LEU:HD23	1:B:80:LEU:HD22	1.93	0.49
1:B:183:PRO:HD2	1:B:269:LEU:O	2.12	0.49
1:B:274:THR:HB	1:B:275:PRO:HD2	1.93	0.49
1:B:87:PRO:HB3	1:B:333:LEU:HD13	1.95	0.49
1:A:207:VAL:HG23	1:A:225:ILE:HD11	1.94	0.48
1:D:127:LYS:HD2	1:D:174:GLU:HG3	1.95	0.48
1:A:241:LEU:HD21	1:A:277:LEU:HD22	1.96	0.48
1:B:116:PRO:HB2	1:B:173:GLN:HG2	1.95	0.48
1:E:152:TRP:HH2	1:E:165:GLU:H	1.59	0.48
1:F:100:ASP:HB3	1:F:103:LEU:HB2	1.96	0.48
1:F:183:PRO:HD2	1:F:269:LEU:O	2.14	0.48
1:C:16:ILE:HD11	1:C:288:ILE:HG21	1.96	0.47
1:C:76:LEU:HB3	1:C:80:LEU:HD22	1.95	0.47
1:D:203:TYR:CZ	1:F:179:VAL:HB	2.49	0.47
1:D:100:ASP:HB3	1:D:103:LEU:HB2	1.97	0.47
1:E:207:VAL:HG23	1:E:225:ILE:HD11	1.96	0.47
1:E:266:PRO:HG3	1:E:316:ILE:HD11	1.97	0.47
1:B:147:ASP:HB2	1:B:148:PRO:HD2	1.96	0.47
1:E:235:ILE:HG22	1:F:233:ILE:HG12	1.97	0.47
1:E:54:TYR:OH	1:E:84:MET:HB2	2.14	0.47
1:F:54:TYR:OH	1:F:84:MET:HB2	2.15	0.47
1:F:326:ASN:N	1:F:326:ASN:HD22	2.13	0.47
1:B:54:TYR:OH	1:B:84:MET:HB2	2.16	0.46
1:A:177:LEU:HD13	1:B:213:ILE:HD11	1.97	0.46
1:C:54:TYR:HB2	1:C:76:LEU:CD2	2.46	0.45
1:C:54:TYR:OH	1:C:84:MET:HB2	2.17	0.45
1:A:167:LEU:O	1:A:170:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:HD21	1:C:277:LEU:HD22	1.99	0.45
1:E:179:VAL:HB	1:F:203:TYR:CZ	2.52	0.45
1:A:116:PRO:HB2	1:A:173:GLN:HG2	1.99	0.44
1:E:7:THR:OG1	1:E:69:THR:HG23	2.17	0.44
1:D:183:PRO:HD2	1:D:269:LEU:O	2.19	0.43
1:D:76:LEU:HD23	1:D:80:LEU:HD22	2.00	0.43
1:C:100:ASP:HB3	1:C:103:LEU:HB2	2.01	0.43
1:C:207:VAL:HG23	1:C:225:ILE:HD11	2.00	0.43
1:D:7:THR:OG1	1:D:69:THR:HG23	2.19	0.43
1:C:183:PRO:HD2	1:C:269:LEU:O	2.19	0.42
1:E:241:LEU:HD21	1:E:277:LEU:HD22	2.00	0.42
1:B:147:ASP:HB2	1:B:148:PRO:CD	2.49	0.42
1:D:114:ARG:NH2	1:D:278:GLU:HG2	2.33	0.42
1:B:207:VAL:HG23	1:B:225:ILE:HD11	2.02	0.42
1:D:201:ARG:NH2	1:E:212:ARG:HD2	2.34	0.42
1:C:71:SER:HB2	1:C:75:HIS:CD2	2.54	0.42
1:B:152:TRP:CG	1:B:163:ARG:HG3	2.55	0.41
1:E:11:HIS:NE2	2:E:402:PO4:O1	2.41	0.41
1:B:165:GLU:HB3	1:B:166:ASP:H	1.68	0.41
1:D:87:PRO:HB3	1:D:333:LEU:HD13	2.02	0.41
1:D:266:PRO:HG3	1:D:316:ILE:HD11	2.02	0.41
1:F:82:GLU:HA	1:F:92:LYS:HD2	2.02	0.41
1:B:7:THR:OG1	1:B:69:THR:HG23	2.21	0.41
1:D:11:HIS:CE1	1:D:70:GLY:HA3	2.55	0.41
1:B:133:PRO:HA	1:B:170:ILE:HG22	2.02	0.41
1:B:17:LEU:HD22	1:B:27:THR:HB	2.03	0.41
1:A:266:PRO:HG3	1:A:316:ILE:HD11	2.03	0.41
1:F:67:VAL:HA	1:F:68:PRO:HD3	1.96	0.41
1:B:168:LYS:H	1:B:168:LYS:HD2	1.86	0.40
1:E:98:GLU:HA	1:E:104:GLU:OE1	2.21	0.40
1:F:56:GLU:HG3	1:F:86:VAL:HG23	2.03	0.40
1:A:324:ILE:HG12	1:A:329:LEU:HD22	2.04	0.40
1:A:179:VAL:HB	1:B:203:TYR:CZ	2.56	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	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
1	B	332/334 (99%)	317 (96%)	15 (4%)	0	100	100
1	C	332/334 (99%)	320 (96%)	10 (3%)	2 (1%)	28	34
1	D	332/334 (99%)	320 (96%)	12 (4%)	0	100	100
1	E	332/334 (99%)	318 (96%)	13 (4%)	1 (0%)	44	55
1	F	332/334 (99%)	319 (96%)	13 (4%)	0	100	100
All	All	1992/2004 (99%)	1916 (96%)	73 (4%)	3 (0%)	51	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	169	ASN
1	C	168	LYS
1	E	135	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	A	290/290 (100%)	281 (97%)	9 (3%)	45	61
1	B	290/290 (100%)	280 (97%)	10 (3%)	42	57
1	C	290/290 (100%)	280 (97%)	10 (3%)	42	57
1	D	290/290 (100%)	279 (96%)	11 (4%)	38	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	290/290 (100%)	279 (96%)	11 (4%)	38	52
1	F	290/290 (100%)	282 (97%)	8 (3%)	49	65
All	All	1740/1740 (100%)	1681 (97%)	59 (3%)	42	57

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	140	LYS
1	A	149	GLU
1	A	156	GLU
1	A	163	ARG
1	A	166	ASP
1	A	200	ASP
1	A	220	GLU
1	A	258	GLU
1	B	21	LYS
1	B	103	LEU
1	B	156	GLU
1	B	168	LYS
1	B	169	ASN
1	B	193	GLU
1	B	200	ASP
1	B	226	THR
1	B	244	ASP
1	B	284	ILE
1	C	21	LYS
1	C	88	TYR
1	C	96	ARG
1	C	103	LEU
1	C	168	LYS
1	C	169	ASN
1	C	170	ILE
1	C	191	ARG
1	C	193	GLU
1	C	200	ASP
1	D	21	LYS
1	D	114	ARG
1	D	137	LYS
1	D	156	GLU
1	D	164	LYS

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Mol	Chain	Res	Type
1	D	169	ASN
1	D	193	GLU
1	D	200	ASP
1	D	220	GLU
1	D	224	ASP
1	D	244	ASP
1	E	21	LYS
1	E	80	LEU
1	E	103	LEU
1	E	137	LYS
1	E	153	ARG
1	E	168	LYS
1	E	169	ASN
1	E	193	GLU
1	E	200	ASP
1	E	219	LEU
1	E	258	GLU
1	F	2	LYS
1	F	103	LEU
1	F	166	ASP
1	F	168	LYS
1	F	169	ASN
1	F	200	ASP
1	F	223	MET
1	F	326	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	171	GLN
1	A	232	ASN
1	A	326	ASN
1	B	83	ASN
1	B	134	HIS
1	B	169	ASN
1	B	171	GLN
1	B	232	ASN
1	C	169	ASN
1	C	171	GLN
1	C	232	ASN
1	D	171	GLN

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Mol	Chain	Res	Type
1	D	232	ASN
1	E	75	HIS
1	E	134	HIS
1	E	169	ASN
1	E	171	GLN
1	E	232	ASN
1	F	75	HIS
1	F	134	HIS
1	F	169	ASN
1	F	171	GLN
1	F	232	ASN
1	F	326	ASN

### 5.3.3 RNA [i](#)

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

25 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	$\# Z  > 2$
3	ADP	A	400	-	25,29,29	1.05	2 (8%)	24,45,45	1.69	2 (8%)
2	PO4	A	401	-	4,4,4	0.79	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	A	402	-	4,4,4	0.84	0	6,6,6	0.42	0
2	PO4	A	501	-	4,4,4	0.73	0	6,6,6	0.35	0
3	ADP	B	400	-	25,29,29	0.99	1 (4%)	24,45,45	1.71	3 (12%)
2	PO4	B	401	-	4,4,4	0.75	0	6,6,6	0.48	0
2	PO4	B	402	-	4,4,4	0.83	0	6,6,6	0.35	0
2	PO4	B	501	-	4,4,4	0.76	0	6,6,6	0.32	0
3	ADP	C	400	-	25,29,29	1.02	1 (4%)	24,45,45	1.67	2 (8%)
2	PO4	C	401	-	4,4,4	0.78	0	6,6,6	0.44	0
2	PO4	C	402	-	4,4,4	0.85	0	6,6,6	0.40	0
2	PO4	C	500	-	4,4,4	0.75	0	6,6,6	0.40	0
2	PO4	C	501	-	4,4,4	0.75	0	6,6,6	0.38	0
3	ADP	D	400	-	25,29,29	1.09	1 (4%)	24,45,45	1.70	3 (12%)
2	PO4	D	401	-	4,4,4	0.74	0	6,6,6	0.45	0
2	PO4	D	402	-	4,4,4	0.80	0	6,6,6	0.42	0
2	PO4	D	501	-	4,4,4	0.77	0	6,6,6	0.36	0
3	ADP	E	400	-	25,29,29	1.06	1 (4%)	24,45,45	1.69	2 (8%)
2	PO4	E	401	-	4,4,4	0.75	0	6,6,6	0.55	0
2	PO4	E	402	-	4,4,4	0.84	0	6,6,6	0.43	0
2	PO4	E	501	-	4,4,4	0.73	0	6,6,6	0.37	0
3	ADP	F	400	-	25,29,29	1.02	1 (4%)	24,45,45	1.66	2 (8%)
2	PO4	F	401	-	4,4,4	0.78	0	6,6,6	0.35	0
2	PO4	F	402	-	4,4,4	0.82	0	6,6,6	0.37	0
2	PO4	F	501	-	4,4,4	0.75	0	6,6,6	0.41	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
3	ADP	A	400	-	-	0/12/32/32	0/3/3/3
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
2	PO4	A	402	-	-	0/0/0/0	0/0/0/0
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
3	ADP	B	400	-	-	0/12/32/32	0/3/3/3
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	402	-	-	0/0/0/0	0/0/0/0
2	PO4	B	501	-	-	0/0/0/0	0/0/0/0
3	ADP	C	400	-	-	0/12/32/32	0/3/3/3
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	PO4	C	402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	C	500	-	-	0/0/0/0	0/0/0/0
2	PO4	C	501	-	-	0/0/0/0	0/0/0/0
3	ADP	D	400	-	-	0/12/32/32	0/3/3/3
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
2	PO4	D	402	-	-	0/0/0/0	0/0/0/0
2	PO4	D	501	-	-	0/0/0/0	0/0/0/0
3	ADP	E	400	-	-	0/12/32/32	0/3/3/3
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
2	PO4	E	402	-	-	0/0/0/0	0/0/0/0
2	PO4	E	501	-	-	0/0/0/0	0/0/0/0
3	ADP	F	400	-	-	0/12/32/32	0/3/3/3
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0
2	PO4	F	402	-	-	0/0/0/0	0/0/0/0
2	PO4	F	501	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ADP	O4'-C1'	2.16	1.44	1.41
3	F	400	ADP	C5-C4	3.01	1.47	1.40
3	B	400	ADP	C5-C4	3.11	1.47	1.40
3	A	400	ADP	C5-C4	3.15	1.47	1.40
3	C	400	ADP	C5-C4	3.17	1.47	1.40
3	D	400	ADP	C5-C4	3.21	1.47	1.40
3	E	400	ADP	C5-C4	3.24	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	ADP	N3-C2-N1	-6.60	123.11	128.86
3	B	400	ADP	N3-C2-N1	-6.53	123.17	128.86
3	A	400	ADP	N3-C2-N1	-6.37	123.31	128.86
3	F	400	ADP	N3-C2-N1	-6.34	123.33	128.86
3	C	400	ADP	N3-C2-N1	-6.31	123.36	128.86
3	E	400	ADP	N3-C2-N1	-6.21	123.45	128.86
3	E	400	ADP	C4-C5-N7	-2.88	106.63	109.41
3	C	400	ADP	C4-C5-N7	-2.85	106.65	109.41
3	A	400	ADP	C4-C5-N7	-2.73	106.78	109.41
3	F	400	ADP	C4-C5-N7	-2.68	106.82	109.41
3	B	400	ADP	C4-C5-N7	-2.55	106.94	109.41
3	D	400	ADP	C4-C5-N7	-2.54	106.95	109.41
3	B	400	ADP	C2-N1-C6	2.04	122.34	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	ADP	C2-N1-C6	2.06	122.37	118.77

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	E	402	PO4	1	0

## 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	334/334 (100%)	0.20	14 (4%)	37 44	8, 18, 40, 54	0
1	B	334/334 (100%)	0.18	20 (5%)	23 29	10, 19, 42, 52	0
1	C	334/334 (100%)	0.13	10 (2%)	51 58	9, 18, 39, 52	0
1	D	334/334 (100%)	0.33	27 (8%)	13 17	10, 20, 42, 54	0
1	E	334/334 (100%)	0.20	21 (6%)	21 27	9, 18, 43, 52	0
1	F	334/334 (100%)	0.18	18 (5%)	26 33	10, 20, 39, 54	0
All	All	2004/2004 (100%)	0.21	110 (5%)	26 32	8, 19, 41, 54	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	135	GLY	5.6
1	E	136	ALA	5.1
1	D	149	GLU	5.1
1	B	166	ASP	5.0
1	E	166	ASP	5.0
1	A	166	ASP	4.8
1	B	165	GLU	4.7
1	A	165	GLU	4.5
1	B	158	PHE	4.3
1	C	169	ASN	4.1
1	C	166	ASP	4.0
1	B	169	ASN	4.0
1	E	165	GLU	3.9
1	E	158	PHE	3.9
1	D	124	ASP	3.9
1	F	224	ASP	3.9
1	E	168	LYS	3.8
1	A	224	ASP	3.7
1	E	134	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	169	ASN	3.7
1	A	169	ASN	3.7
1	D	161	ILE	3.6
1	F	70	GLY	3.6
1	D	164	LYS	3.6
1	F	165	GLU	3.6
1	A	135	GLY	3.5
1	D	126	GLU	3.5
1	D	118	VAL	3.5
1	E	161	ILE	3.4
1	B	222	ASP	3.4
1	D	160	GLY	3.4
1	D	163	ARG	3.3
1	C	165	GLU	3.3
1	B	164	LYS	3.3
1	B	160	GLY	3.2
1	A	222	ASP	3.2
1	E	153	ARG	3.2
1	F	163	ARG	3.2
1	F	222	ASP	3.2
1	B	162	LYS	3.1
1	D	156	GLU	3.1
1	F	166	ASP	3.0
1	B	138	GLY	3.0
1	B	156	GLU	3.0
1	E	156	GLU	3.0
1	A	76	LEU	2.9
1	F	149	GLU	2.9
1	E	222	ASP	2.8
1	E	224	ASP	2.8
1	A	134	HIS	2.8
1	B	161	ILE	2.8
1	E	139	GLY	2.8
1	F	134	HIS	2.7
1	D	123	ASP	2.7
1	D	153	ARG	2.7
1	F	233	ILE	2.7
1	F	124	ASP	2.7
1	D	224	ASP	2.7
1	D	158	PHE	2.7
1	D	165	GLU	2.6
1	D	222	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	126	GLU	2.6
1	B	159	LEU	2.6
1	D	152	TRP	2.6
1	A	161	ILE	2.6
1	D	148	PRO	2.5
1	E	162	LYS	2.5
1	D	125	ILE	2.5
1	D	134	HIS	2.5
1	F	135	GLY	2.5
1	C	168	LYS	2.5
1	D	162	LYS	2.5
1	E	120	GLU	2.5
1	B	163	ARG	2.5
1	D	120	GLU	2.4
1	C	222	ASP	2.4
1	B	75	HIS	2.4
1	A	75	HIS	2.3
1	F	123	ASP	2.3
1	A	158	PHE	2.3
1	B	167	LEU	2.3
1	E	155	ALA	2.3
1	B	137	LYS	2.3
1	F	162	LYS	2.3
1	A	168	LYS	2.2
1	F	169	ASN	2.2
1	F	161	ILE	2.2
1	B	80	LEU	2.2
1	E	157	LYS	2.2
1	B	134	HIS	2.2
1	A	163	ARG	2.2
1	C	136	ALA	2.2
1	F	146	LYS	2.1
1	D	234	PRO	2.1
1	C	75	HIS	2.1
1	B	135	GLY	2.1
1	F	234	PRO	2.1
1	C	219	LEU	2.1
1	D	166	ASP	2.1
1	B	149	GLU	2.1
1	F	126	GLU	2.1
1	E	164	LYS	2.1
1	C	156	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	123	ASP	2.0
1	D	233	ILE	2.0
1	D	119	TYR	2.0
1	A	156	GLU	2.0
1	E	235	ILE	2.0
1	C	162	LYS	2.0
1	D	136	ALA	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	A	501	5/5	0.94	0.22	2.81	43,44,44,44	0
2	PO4	B	501	5/5	0.94	0.17	1.94	38,39,40,40	0
3	ADP	F	400	27/27	0.85	0.19	0.71	18,22,45,45	0
2	PO4	F	501	5/5	0.94	0.15	0.53	46,47,47,47	0
3	ADP	C	400	27/27	0.88	0.18	0.46	19,23,44,45	0
3	ADP	A	400	27/27	0.86	0.17	0.28	16,19,42,42	0
3	ADP	D	400	27/27	0.84	0.18	0.26	22,25,45,45	0
3	ADP	B	400	27/27	0.85	0.17	0.18	24,27,45,45	0
3	ADP	E	400	27/27	0.84	0.19	0.18	22,26,47,48	0
2	PO4	E	402	5/5	0.98	0.16	0.11	22,23,24,24	0
2	PO4	B	401	5/5	0.94	0.17	0.08	37,37,37,38	0
2	PO4	C	401	5/5	0.95	0.14	-0.49	36,37,37,38	0
2	PO4	A	401	5/5	0.94	0.12	-0.51	39,39,39,39	0
2	PO4	E	401	5/5	0.95	0.12	-0.63	39,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	D	402	5/5	0.98	0.14	-0.75	21,22,23,23	0
2	PO4	D	401	5/5	0.96	0.12	-0.76	36,37,37,37	0
2	PO4	F	402	5/5	0.98	0.13	-0.79	17,18,18,18	0
2	PO4	A	402	5/5	0.99	0.12	-0.90	16,16,17,17	0
2	PO4	F	401	5/5	0.96	0.12	-1.00	40,40,41,41	0
2	PO4	C	500	5/5	0.97	0.11	-1.04	32,33,33,33	0
2	PO4	C	402	5/5	0.98	0.13	-1.10	18,18,19,20	0
2	PO4	B	402	5/5	0.99	0.12	-1.96	17,17,18,19	0
2	PO4	D	501	5/5	0.89	0.23	-	57,57,58,58	0
2	PO4	C	501	5/5	0.97	0.14	-	37,37,37,37	0
2	PO4	E	501	5/5	0.96	0.18	-	50,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.