



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2017 – 04:12 PM EDT

PDB ID : 5DW3  
Title : Tryptophan Synthase beta-subunit from *Pyrococcus furiosus* with product L-tryptophan non-covalently bound in the active site  
Authors : Buller, A.R.; Arnold, F.H.  
Deposited on : unknown  
Resolution : 1.74 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-20029824  
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-20029824

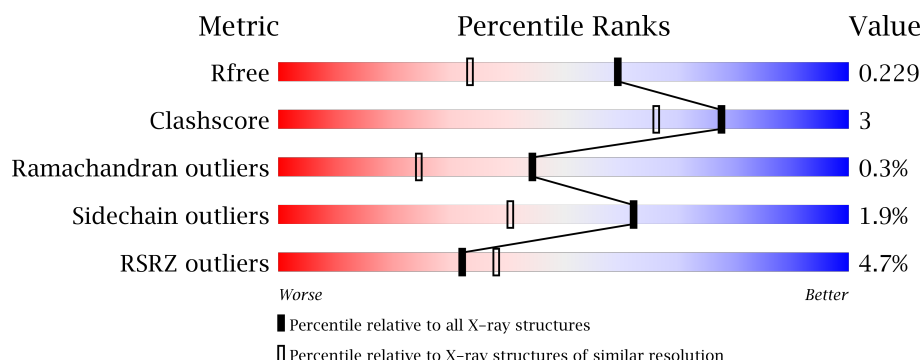
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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	396	<div> <div>0.1%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	B	396	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	396	<div> <div>6%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	D	396	<div> <div>9%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRP	C	402	-	-	-	X
3	TRP	D	402[A]	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12060 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 Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	P	S	0	1	0
			2930	1873	500	544	1	12			
1	B	386	Total	C	N	O	P	S	0	2	0
			2976	1898	515	550	1	12			
1	C	384	Total	C	N	O	P	S	0	1	0
			2914	1862	496	543	1	12			
1	D	384	Total	C	N	O	P	S	0	0	0
			2865	1830	489	533	1	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	LEU	-	expression tag	UNP Q8U093
A	390	GLU	-	expression tag	UNP Q8U093
A	391	HIS	-	expression tag	UNP Q8U093
A	392	HIS	-	expression tag	UNP Q8U093
A	393	HIS	-	expression tag	UNP Q8U093
A	394	HIS	-	expression tag	UNP Q8U093
A	395	HIS	-	expression tag	UNP Q8U093
A	396	HIS	-	expression tag	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	UNP Q8U093
C	389	LEU	-	expression tag	UNP Q8U093
C	390	GLU	-	expression tag	UNP Q8U093
C	391	HIS	-	expression tag	UNP Q8U093
C	392	HIS	-	expression tag	UNP Q8U093
C	393	HIS	-	expression tag	UNP Q8U093

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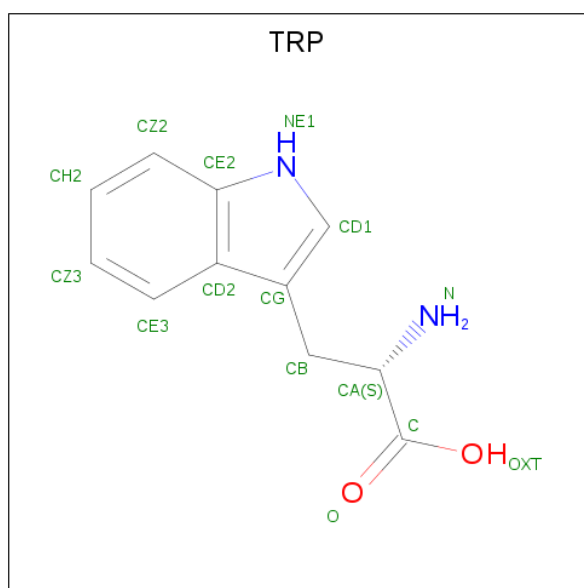
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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP Q8U093
C	395	HIS	-	expression tag	UNP Q8U093
C	396	HIS	-	expression tag	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093
D	392	HIS	-	expression tag	UNP Q8U093
D	393	HIS	-	expression tag	UNP Q8U093
D	394	HIS	-	expression tag	UNP Q8U093
D	395	HIS	-	expression tag	UNP Q8U093
D	396	HIS	-	expression tag	UNP Q8U093

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

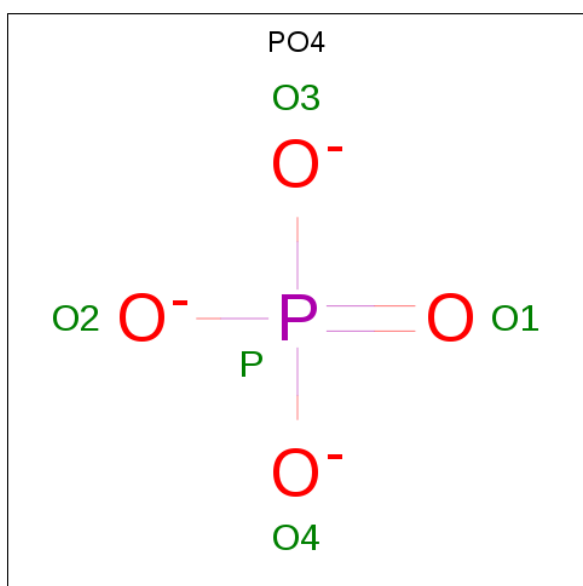
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	1
			15	11	2	2		

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



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

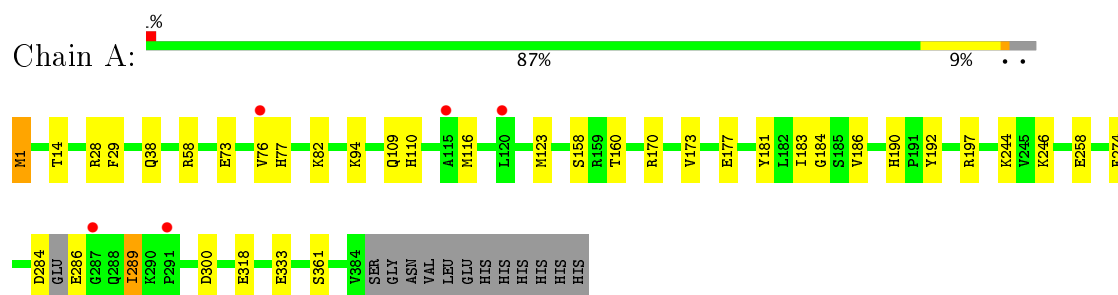
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103	103		
5	B	94	Total	O	0	2
			94	94		
5	C	51	Total	O	0	0
			51	51		
5	D	53	Total	O	0	0
			53	53		

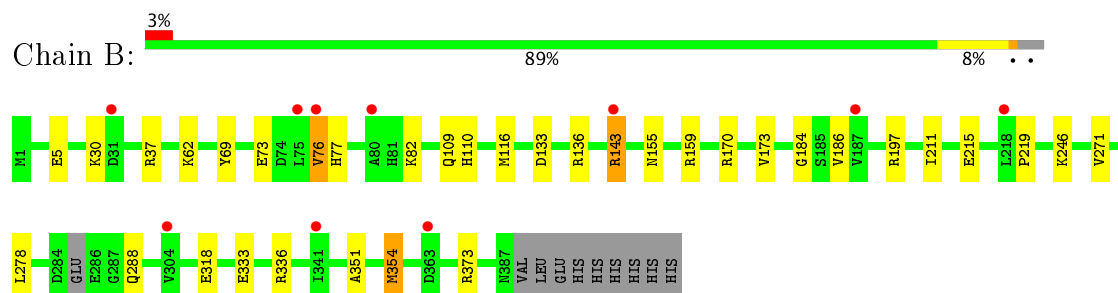
### 3 Residue-property plots [i](#)

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.

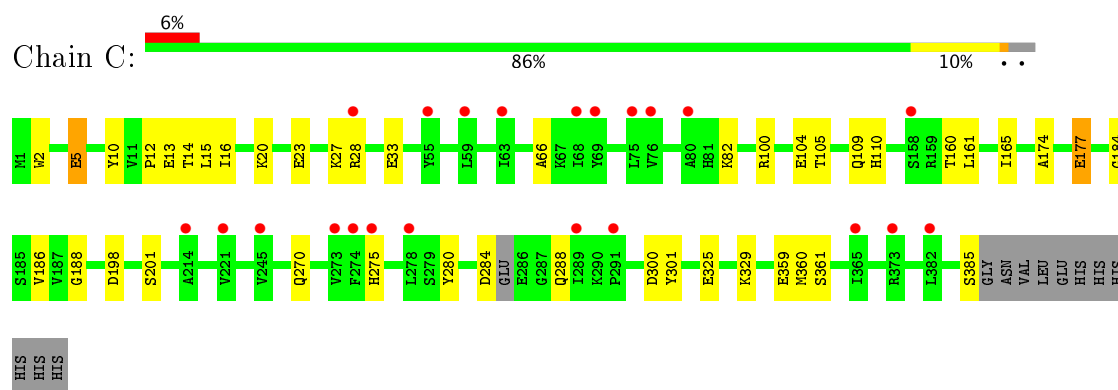
- Molecule 1: Tryptophan synthase beta chain 1



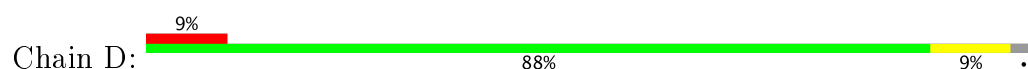
- Molecule 1: Tryptophan synthase beta chain 1

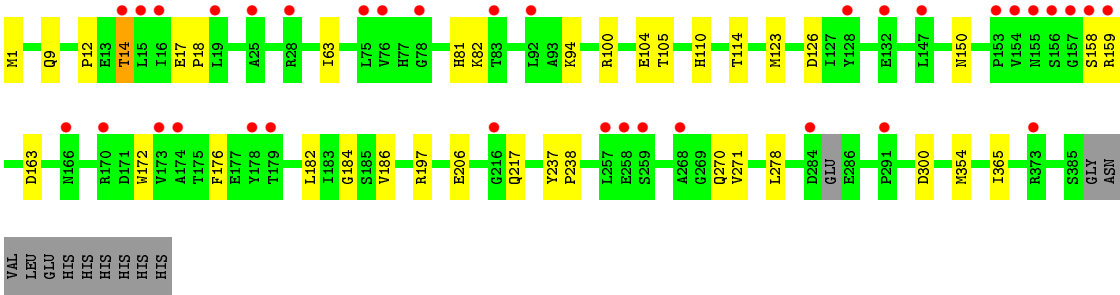


- Molecule 1: Tryptophan synthase beta chain 1



- Molecule 1: Tryptophan synthase beta chain 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.74Å 108.93Å 160.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.74 39.08 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-1.74) 98.4 (39.08-1.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.185 , 0.224 0.193 , 0.229	Depositor DCC
$R_{free}$ test set	7347 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% 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: NA, PO4, LLP

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	0.97	0/2968	0.94	2/4014 (0.0%)
1	B	1.00	1/3014 (0.0%)	0.98	9/4072 (0.2%)
1	C	1.03	4/2953 (0.1%)	0.94	2/4002 (0.0%)
1	D	0.94	2/2898 (0.1%)	0.91	3/3928 (0.1%)
All	All	0.98	7/11833 (0.1%)	0.94	16/16016 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	GLU	CD-OE1	7.44	1.33	1.25
1	D	206	GLU	CD-OE1	6.86	1.33	1.25
1	C	5	GLU	CD-OE1	6.47	1.32	1.25
1	C	201	SER	CB-OG	-5.84	1.34	1.42
1	C	280	TYR	CB-CG	-5.79	1.43	1.51
1	C	104	GLU	CD-OE2	5.44	1.31	1.25
1	D	104	GLU	CD-OE1	5.20	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	336	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	143[A]	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	143[B]	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	373	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	197	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	D	197	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	354	MET	CG-SD-CE	5.85	109.57	100.20
1	C	100	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	58	ARG	NE-CZ-NH2	-5.53	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	D	197	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	D	100	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	76	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	C	198	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	197	ARG	NE-CZ-NH2	5.01	122.81	120.30

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	2930	0	2896	21	0
1	B	2976	0	2956	18	0
1	C	2914	0	2839	23	0
1	D	2865	0	2772	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	9	1	0
3	B	15	0	9	0	0
3	C	15	0	9	2	0
3	D	15	0	9	1	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
5	A	103	0	0	2	0
5	B	94	0	0	4	0
5	C	51	0	0	0	0
5	D	53	0	0	1	0
All	All	12060	0	11499	78	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 (78) 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:246:LYS:NZ	1:A:318:GLU:OE1	2.18	0.77
1:C:105:THR:HA	4:C:403[B]:PO4:O2	1.87	0.73
1:C:109:GLN:HB2	3:C:402:TRP:O	1.93	0.69
1:B:73:GLU:O	1:B:76:VAL:HG12	1.95	0.65
1:D:94:LYS:HB2	1:D:123:MET:HE1	1.80	0.62
1:D:63:ILE:HD11	1:D:354:MET:HG2	1.82	0.62
1:C:177:GLU:CD	1:C:177:GLU:H	2.04	0.61
1:D:217:GLN:HE21	1:D:365:ILE:HD12	1.65	0.60
1:C:16:ILE:O	1:C:20:LYS:HG2	2.00	0.60
1:C:359:GLU:O	1:C:360:MET:HG3	2.04	0.58
1:C:165:ILE:HG21	1:C:275[A]:HIS:CD2	2.39	0.58
1:A:170:ARG:O	1:A:173:VAL:HG22	2.05	0.57
1:B:109[B]:GLN:HG2	5:B:509:HOH:O	2.04	0.57
1:B:143[B]:ARG:NH1	5:B:501:HOH:O	2.18	0.56
1:A:181:TYR:CZ	1:A:183:ILE:HG12	2.42	0.55
1:C:12:PRO:HB2	1:C:14:THR:HG22	1.88	0.55
1:B:77:HIS:NE2	1:B:116:MET:CE	2.70	0.54
1:B:133:ASP:OD1	1:B:136:ARG:NH2	2.39	0.54
1:A:177:GLU:CD	1:A:177:GLU:H	2.11	0.53
1:D:172:TRP:O	1:D:176:PHE:HB3	2.09	0.53
1:A:77:HIS:CD2	1:A:116:MET:CE	2.93	0.52
1:D:12:PRO:HG2	1:D:14:THR:HG23	1.92	0.52
1:A:181:TYR:CE2	1:A:183:ILE:HD11	2.44	0.52
1:A:94:LYS:HB2	1:A:123:MET:CE	2.40	0.51
1:C:325:GLU:O	1:C:329:LYS:HG3	2.10	0.51
1:A:177:GLU:HG2	5:A:594:HOH:O	2.10	0.51
1:A:300:ASP:C	1:A:300:ASP:OD1	2.47	0.51
1:D:82:LLP:HE2	5:D:521:HOH:O	2.11	0.50
1:C:66:ALA:HA	1:C:361:SER:O	2.12	0.49
1:C:110:HIS:CE1	1:C:184:GLY:HA2	2.47	0.49
1:B:271:VAL:CG1	1:B:278:LEU:HD11	2.43	0.48
1:D:271:VAL:HG12	1:D:278:LEU:HD11	1.96	0.48
1:A:284:ASP:OD1	1:A:286:GLU:N	2.46	0.47
1:C:174:ALA:O	1:C:177:GLU:OE2	2.31	0.47
1:D:114:THR:HG23	1:D:182:LEU:HD13	1.97	0.47
1:D:82:LLP:HE3	3:D:402[A]:TRP:HB2	1.95	0.46
1:D:126:ASP:OD1	1:D:150:ASN:HB2	2.15	0.46
1:A:28:ARG:HD3	1:A:29:PHE:CZ	2.50	0.46
1:A:1:MET:HA	1:A:190:HIS:ND1	2.31	0.46
1:C:82:LLP:O3	1:C:82:LLP:NZ	2.49	0.45
1:C:23:GLU:HG2	1:C:27:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:TYR:HB3	1:D:238:PRO:HD3	1.99	0.45
1:A:274:PHE:CD2	1:A:289:ILE:HD12	2.51	0.45
1:B:110:HIS:CE1	1:B:184:GLY:HA2	2.52	0.45
1:C:165:ILE:CG2	1:C:275[A]:HIS:CD2	2.99	0.45
1:A:109:GLN:HB2	3:A:402:TRP:OXT	2.17	0.45
1:C:2:TRP:HH2	1:C:10:TYR:HH	1.64	0.45
1:B:211:ILE:HG21	1:B:219:PRO:HD3	1.99	0.44
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.52	0.44
1:B:246:LYS:NZ	1:B:318:GLU:OE1	2.47	0.44
1:A:82:LLP:HE2	5:A:539:HOH:O	2.18	0.43
1:B:69:TYR:OH	1:B:215:GLU:OE2	2.29	0.43
1:C:165:ILE:HG21	1:C:275[A]:HIS:CG	2.52	0.43
1:B:82:LLP:HE2	5:B:515:HOH:O	2.19	0.43
1:B:143[B]:ARG:NE	5:B:501:HOH:O	2.48	0.43
1:C:284:ASP:N	1:C:288:GLN:O	2.41	0.43
1:A:158:SER:O	1:A:160:THR:HG23	2.19	0.43
1:D:1:MET:HE3	1:D:9:GLN:N	2.33	0.43
1:B:351:ALA:HA	1:B:354:MET:HE2	2.01	0.42
1:A:183:ILE:HD12	1:A:192:TYR:CD2	2.55	0.42
1:C:12:PRO:HD2	1:C:15:LEU:HD12	2.00	0.42
1:D:110:HIS:CE1	1:D:184:GLY:HA2	2.55	0.42
1:A:73:GLU:O	1:A:76:VAL:HG12	2.20	0.42
1:D:81:HIS:O	1:D:82:LLP:C	2.67	0.42
1:A:38:GLN:NE2	1:C:33:GLU:OE1	2.53	0.41
1:C:160:THR:OG1	1:C:161:LEU:N	2.50	0.41
1:B:170:ARG:O	1:B:173:VAL:HG22	2.20	0.41
1:B:77:HIS:NE2	1:B:116:MET:HE2	2.36	0.41
1:C:82:LLP:HD2	1:C:110:HIS:HA	2.03	0.41
1:D:82:LLP:O3	1:D:82:LLP:NZ	2.53	0.41
1:B:155:ASN:HA	1:B:159:ARG:HG2	2.02	0.41
1:D:17:GLU:N	1:D:18:PRO:HD2	2.36	0.41
1:B:82:LLP:O3	1:B:82:LLP:NZ	2.54	0.40
1:A:181:TYR:CE2	1:A:183:ILE:CG1	3.05	0.40
1:B:62:LYS:NZ	1:B:333:GLU:OE2	2.37	0.40
1:C:301:TYR:HB2	3:C:402:TRP:CZ3	2.57	0.40
1:D:105:THR:OG1	4:D:403[B]:PO4:O3	2.25	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	379/396 (96%)	368 (97%)	10 (3%)	1 (0%)	44	24
1	B	383/396 (97%)	375 (98%)	7 (2%)	1 (0%)	44	24
1	C	380/396 (96%)	370 (97%)	8 (2%)	2 (0%)	32	13
1	D	379/396 (96%)	369 (97%)	9 (2%)	1 (0%)	44	24
All	All	1521/1584 (96%)	1482 (97%)	34 (2%)	5 (0%)	44	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	GLU
1	C	186	VAL
1	D	186	VAL
1	A	186	VAL
1	B	186	VAL

### 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	292/315 (93%)	285 (98%)	7 (2%)	54	30
1	B	298/315 (95%)	296 (99%)	2 (1%)	87	78
1	C	286/315 (91%)	280 (98%)	6 (2%)	59	35
1	D	274/315 (87%)	268 (98%)	6 (2%)	57	33
All	All	1150/1260 (91%)	1129 (98%)	21 (2%)	62	44

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	THR
1	A	244	LYS
1	A	258	GLU
1	A	289	ILE
1	A	333	GLU
1	A	361	SER
1	B	30	LYS
1	B	288	GLN
1	C	5	GLU
1	C	28	ARG
1	C	177	GLU
1	C	270	GLN
1	C	300	ASP
1	C	385	SER
1	D	14	THR
1	D	158	SER
1	D	159	ARG
1	D	163	ASP
1	D	270	GLN
1	D	300	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	217	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	LLP	A	82	1	24,24,25	2.71	5 (20%)	28,32,34	1.76	9 (32%)
1	LLP	B	82	1	24,24,25	2.00	7 (29%)	28,32,34	1.75	8 (28%)
1	LLP	C	82	1	24,24,25	2.45	7 (29%)	28,32,34	1.73	10 (35%)
1	LLP	D	82	1	24,24,25	2.08	6 (25%)	28,32,34	1.42	4 (14%)

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	LLP	A	82	1	-	0/15/17/19	0/1/1/1
1	LLP	B	82	1	-	0/15/17/19	0/1/1/1
1	LLP	C	82	1	-	0/15/17/19	0/1/1/1
1	LLP	D	82	1	-	0/15/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	LLP	CE-NZ	-2.44	1.41	1.46
1	A	82	LLP	O3-C3	-2.30	1.31	1.37
1	C	82	LLP	O3-C3	-2.21	1.31	1.37
1	D	82	LLP	O3-C3	-2.09	1.32	1.37
1	B	82	LLP	P-OP3	-2.07	1.46	1.54
1	C	82	LLP	CA-C	2.14	1.53	1.50
1	C	82	LLP	C6-C5	2.24	1.42	1.37
1	D	82	LLP	C4-C4'	3.04	1.52	1.46
1	B	82	LLP	C4-C5	3.05	1.45	1.42
1	B	82	LLP	CB-CA	3.08	1.57	1.53
1	B	82	LLP	C4-C3	3.11	1.45	1.40
1	C	82	LLP	C4-C4'	3.13	1.52	1.46
1	A	82	LLP	C4-C5	3.41	1.46	1.42
1	D	82	LLP	C4-C5	3.53	1.46	1.42
1	C	82	LLP	C4'-NZ	3.80	1.38	1.27
1	C	82	LLP	C4-C3	3.99	1.47	1.40
1	D	82	LLP	C3-C2	4.13	1.43	1.40
1	D	82	LLP	C4-C3	4.48	1.48	1.40
1	D	82	LLP	C4'-NZ	4.71	1.41	1.27
1	B	82	LLP	C3-C2	4.73	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	LLP	C4'-NZ	4.93	1.41	1.27
1	A	82	LLP	C4'-NZ	5.03	1.42	1.27
1	A	82	LLP	C4-C3	5.73	1.50	1.40
1	C	82	LLP	C3-C2	8.77	1.46	1.40
1	A	82	LLP	C3-C2	9.30	1.47	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LLP	C4-C4'-NZ	-3.39	108.19	124.66
1	D	82	LLP	C4-C4'-NZ	-3.26	108.82	124.66
1	B	82	LLP	C3-C2-N1	-3.12	116.66	120.75
1	B	82	LLP	C4-C3-C2	-2.98	118.32	120.15
1	C	82	LLP	C3-C2-N1	-2.84	117.03	120.75
1	B	82	LLP	CB-CA-C	-2.66	107.27	111.65
1	A	82	LLP	C4-C3-C2	-2.58	118.57	120.15
1	D	82	LLP	OP3-P-OP4	-2.55	99.94	106.73
1	C	82	LLP	C4-C4'-NZ	-2.51	112.49	124.66
1	C	82	LLP	OP3-P-OP4	-2.34	100.51	106.73
1	A	82	LLP	C2'-C2-C3	-2.34	118.18	120.96
1	A	82	LLP	C3-C2-N1	-2.33	117.69	120.75
1	C	82	LLP	CD-CG-CB	-2.22	105.76	113.63
1	B	82	LLP	C4-C4'-NZ	-2.21	113.91	124.66
1	B	82	LLP	C2'-C2-C3	-2.06	118.50	120.96
1	C	82	LLP	C2'-C2-C3	-2.06	118.51	120.96
1	D	82	LLP	CD-CG-CB	-2.05	106.33	113.63
1	C	82	LLP	C5-C4-C4'	-2.01	118.36	121.36
1	B	82	LLP	OP4-C5'-C5	2.23	113.80	109.32
1	C	82	LLP	OP3-P-OP2	2.23	116.62	107.61
1	D	82	LLP	O3-C3-C2	2.28	122.56	117.78
1	C	82	LLP	OP4-C5'-C5	2.33	114.00	109.32
1	A	82	LLP	C6-N1-C2	2.39	123.87	119.26
1	A	82	LLP	OP4-C5'-C5	2.42	114.19	109.32
1	C	82	LLP	C6-N1-C2	2.49	124.05	119.26
1	A	82	LLP	C5'-C5-C6	2.95	124.40	119.33
1	A	82	LLP	OP3-P-OP1	2.98	122.17	110.50
1	A	82	LLP	C2'-C2-N1	3.12	124.12	117.89
1	C	82	LLP	C2'-C2-N1	3.21	124.31	117.89
1	B	82	LLP	C2'-C2-N1	3.47	124.83	117.89
1	B	82	LLP	C6-N1-C2	3.96	126.88	119.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	82	LLP	1	0
1	B	82	LLP	2	0
1	C	82	LLP	2	0
1	D	82	LLP	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	TRP	A	402	-	11,16,16	0.99	1 (9%)	11,22,22	0.87	0
3	TRP	B	402	-	11,16,16	1.29	2 (18%)	11,22,22	1.01	1 (9%)
3	TRP	C	402	4	11,16,16	1.22	1 (9%)	11,22,22	1.27	2 (18%)
4	PO4	C	403[B]	3	4,4,4	0.99	0	6,6,6	0.51	0
3	TRP	D	402[A]	-	11,16,16	0.65	0	11,22,22	0.85	0
4	PO4	D	403[B]	-	4,4,4	0.80	0	6,6,6	0.43	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	TRP	A	402	-	-	0/3/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	B	402	-	-	0/3/8/8	0/2/2/2
3	TRP	C	402	4	-	0/3/8/8	0/2/2/2
4	PO4	C	403[B]	3	-	0/0/0/0	0/0/0/0
3	TRP	D	402[A]	-	-	0/3/8/8	0/2/2/2
4	PO4	D	403[B]	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	TRP	CB-CG	-2.26	1.44	1.51
3	C	402	TRP	CZ2-CE2	-2.03	1.38	1.41
3	A	402	TRP	CZ3-CE3	2.07	1.41	1.36
3	B	402	TRP	CZ3-CE3	3.09	1.43	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	TRP	CH2-CZ2-CE2	-2.39	116.47	120.07
3	C	402	TRP	CZ3-CE3-CD2	-2.30	117.59	120.88
3	B	402	TRP	CZ3-CE3-CD2	-2.07	117.91	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TRP	1	0
3	C	402	TRP	2	0
4	C	403[B]	PO4	1	0
3	D	402[A]	TRP	1	0
4	D	403[B]	PO4	1	0

## 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	A	382/396 (96%)	0.09	5 (1%) 77 83	24, 37, 57, 93	0
1	B	385/396 (97%)	0.28	10 (2%) 56 63	23, 34, 54, 69	0
1	C	383/396 (96%)	0.37	22 (5%) 24 30	23, 42, 70, 89	1 (0%)
1	D	383/396 (96%)	0.54	35 (9%) 10 12	24, 43, 80, 118	0
All	All	1533/1584 (96%)	0.32	72 (4%) 32 38	23, 39, 68, 118	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	59	LEU	6.1
1	D	157	GLY	5.8
1	D	291	PRO	5.6
1	A	291	PRO	4.9
1	D	15	LEU	4.7
1	D	16	ILE	4.3
1	C	274	PHE	4.2
1	D	156	SER	3.8
1	D	158	SER	3.6
1	C	214	ALA	3.6
1	D	154	VAL	3.5
1	D	173	VAL	3.3
1	D	259	SER	3.3
1	C	75	LEU	3.3
1	D	178	TYR	3.3
1	D	128	TYR	3.3
1	C	278	LEU	3.2
1	D	75	LEU	3.2
1	D	166	ASN	3.0
1	A	287	GLY	2.9
1	C	245	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	257	LEU	2.8
1	D	284	ASP	2.8
1	C	28	ARG	2.7
1	D	159	ARG	2.6
1	D	25	ALA	2.6
1	C	69	TYR	2.6
1	D	268	ALA	2.6
1	D	14	THR	2.6
1	B	304	VAL	2.5
1	B	143[A]	ARG	2.5
1	A	76	VAL	2.5
1	C	365	ILE	2.5
1	B	75	LEU	2.5
1	C	63	ILE	2.4
1	C	76	VAL	2.4
1	C	291	PRO	2.4
1	D	174	ALA	2.4
1	D	83	THR	2.4
1	B	218	LEU	2.3
1	D	153	PRO	2.3
1	C	273	VAL	2.3
1	C	158	SER	2.3
1	D	132	GLU	2.3
1	C	80	ALA	2.3
1	D	76	VAL	2.3
1	D	373	ARG	2.2
1	C	275[A]	HIS	2.2
1	C	373	ARG	2.2
1	C	68	ILE	2.2
1	C	289	ILE	2.2
1	A	115	ALA	2.2
1	B	341	ILE	2.2
1	D	78	GLY	2.2
1	D	216	GLY	2.2
1	A	120	LEU	2.1
1	D	147	LEU	2.1
1	D	258	GLU	2.1
1	B	363	ASP	2.1
1	D	28	ARG	2.1
1	B	80	ALA	2.1
1	B	76	VAL	2.1
1	B	187	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	19	LEU	2.1
1	D	155	ASN	2.0
1	D	170	ARG	2.0
1	B	31	ASP	2.0
1	C	55	TYR	2.0
1	C	221	VAL	2.0
1	C	382	LEU	2.0
1	D	92	LEU	2.0
1	D	179	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	82	24/25	0.96	0.13	-	24,26,29,31	0
1	LLP	D	82	24/25	0.97	0.13	-	27,29,33,35	0
1	LLP	B	82	24/25	0.98	0.18	-	21,24,26,28	0
1	LLP	C	82	24/25	0.98	0.14	-	22,25,26,27	0

## 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
3	TRP	D	402[A]	15/15	0.85	0.43	14.47	39,41,44,46	15
3	TRP	C	402	15/15	0.92	0.23	4.45	29,32,33,33	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	C	403[B]	5/5	0.95	0.15	1.65	29,30,32,35	5
3	TRP	B	402	15/15	0.97	0.15	-0.17	27,29,31,31	0
3	TRP	A	402	15/15	0.95	0.09	-0.18	32,34,36,37	0
4	PO4	D	403[B]	5/5	0.96	0.09	-0.44	51,59,63,64	5
2	NA	B	401	1/1	0.95	0.10	-0.52	35,35,35,35	0
2	NA	C	401	1/1	0.91	0.08	-0.81	37,37,37,37	0
2	NA	A	401	1/1	0.98	0.04	-1.69	39,39,39,39	0
2	NA	D	401	1/1	0.97	0.05	-2.02	41,41,41,41	0

## 6.5 Other polymers

There are no such residues in this entry.