



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:14 pm BST

PDB ID : 1LK7  
Title : Structure of D-Ribose-5-Phosphate Isomerase from in complex with phospho-erythronic acid  
Authors : Ishikawa, K.; Matsui, I.; Payan, F.; Cambillau, C.; Ishida, H.; Kwarabayasi, Y.; Kikuchi, H.; Roussel, A.  
Deposited on : 2002-04-24  
Resolution : 2.00 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 : 2.11  
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) : 2.11

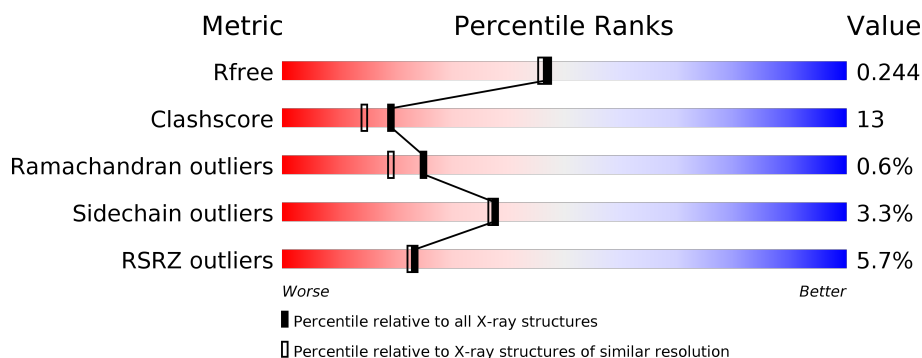
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	229	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>19%</div> </div> <div></div> </div>
1	B	229	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>27%</div> </div> <div></div> </div>
1	C	229	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>17%</div> </div> <div></div> </div>
1	D	229	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> </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
2	CL	D	2004	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7493 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-Ribose-5-Phosphate Isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1756	1125	284	339	8			
1	B	229	Total	C	N	O	S	0	0	0
			1756	1125	284	339	8			
1	C	229	Total	C	N	O	S	0	0	0
			1756	1125	284	339	8			
1	D	229	Total	C	N	O	S	0	0	0
			1756	1125	284	339	8			

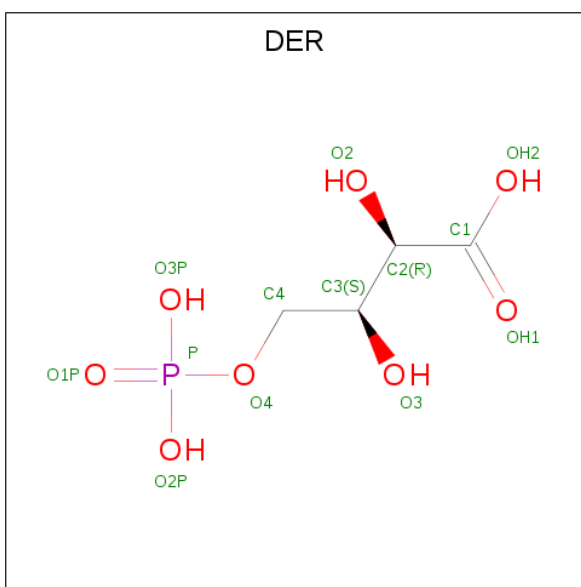
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cl	0	0
			3	3		
2	A	3	Total	Cl	0	0
			3	3		
2	D	2	Total	Cl	0	0
			2	2		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is D-4-PHOSPHOERYTHRNIC ACID (three-letter code: DER) (formula: C<sub>4</sub>H<sub>9</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			13	4	8	1		
4	B	1	Total	C	O	P	0	0
			13	4	8	1		
4	C	1	Total	C	O	P	0	0
			13	4	8	1		
4	D	1	Total	C	O	P	0	0
			13	4	8	1		

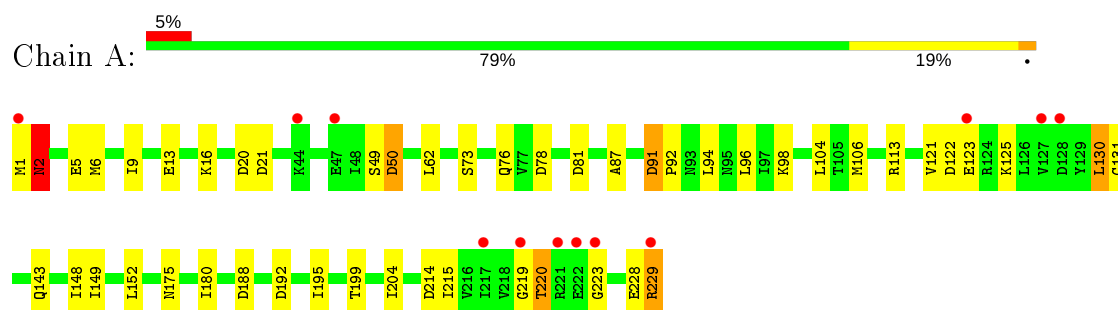
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total	O	0	0
			97	97		
5	B	99	Total	O	0	0
			99	99		
5	C	102	Total	O	0	0
			102	102		
5	D	107	Total	O	0	0
			107	107		

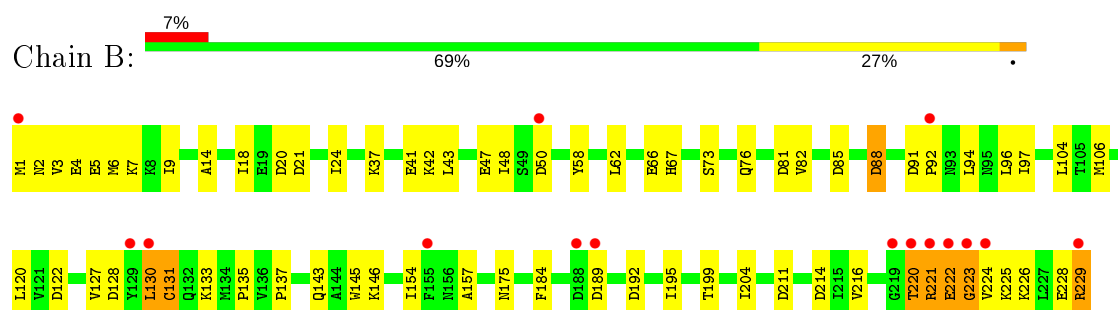
### 3 Residue-property plots [i](#)

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.

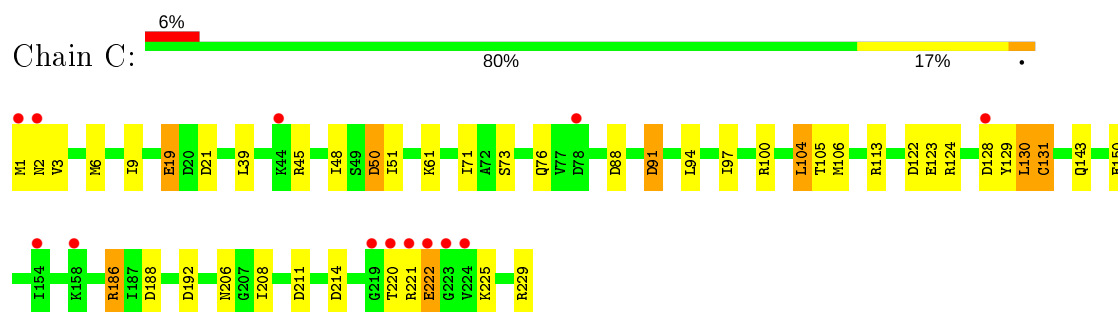
#### • Molecule 1: D-Ribose-5-Phosphate Isomerase



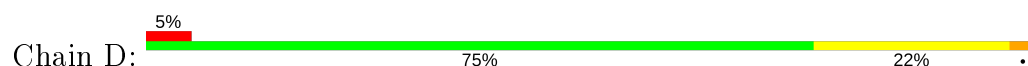
#### • Molecule 1: D-Ribose-5-Phosphate Isomerase

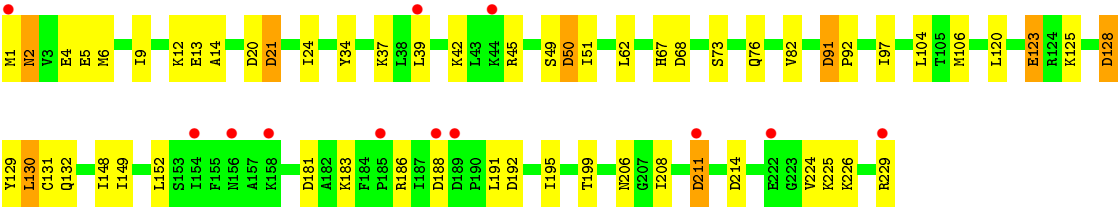


#### • Molecule 1: D-Ribose-5-Phosphate Isomerase



#### • Molecule 1: D-Ribose-5-Phosphate Isomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.69Å 114.92Å 119.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.00) 95.9 (15.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.247 0.206 , 0.244	Depositor DCC
$R_{free}$ test set	3322 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DER, CL

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	0.58	0/1779	0.90	10/2406 (0.4%)
1	B	0.63	0/1779	0.94	11/2406 (0.5%)
1	C	0.57	0/1779	0.89	6/2406 (0.2%)
1	D	0.59	0/1779	0.89	11/2406 (0.5%)
All	All	0.59	0/7116	0.91	38/9624 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	ASP	CB-CG-OD2	8.82	126.24	118.30
1	A	91	ASP	CB-CG-OD2	8.65	126.08	118.30
1	D	91	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	211	ASP	CB-CG-OD2	7.66	125.20	118.30
1	D	50	ASP	CB-CG-OD2	6.87	124.49	118.30
1	B	20	ASP	CB-CG-OD2	6.41	124.06	118.30
1	A	21	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	81	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	50	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	128	ASP	CB-CG-OD2	6.22	123.89	118.30
1	B	122	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	20	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	128	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	188	ASP	CB-CG-OD2	5.97	123.67	118.30
1	D	128	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	21	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	122	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	50	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	214	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	192	ASP	CB-CG-OD2	5.75	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	50	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	78	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	81	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	192	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	211	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	188	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	214	ASP	CB-CG-OD2	5.34	123.10	118.30
1	D	68	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	181	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	192	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	88	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	214	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	85	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	122	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	189	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	192	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	20	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1756	0	1814	34	0
1	B	1756	0	1814	69	0
1	C	1756	0	1814	48	0
1	D	1756	0	1814	42	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	0	6	1	0
4	C	13	0	6	1	0
4	D	13	0	6	2	0
5	A	97	0	0	5	0
5	B	99	0	0	19	0
5	C	102	0	0	11	0
5	D	107	0	0	7	0
All	All	7493	0	7280	185	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 13.

All (185) 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:6:MET:SD	5:B:2096:HOH:O	1.93	1.25
2:D:2004:CL:CL	4:D:1004:DER:OH2	2.01	1.15
1:A:143:GLN:NE2	1:B:106:MET:SD	2.26	1.08
1:B:226:LYS:N	5:B:2100:HOH:O	2.06	0.88
1:D:21:ASP:OD2	1:D:50:ASP:OD1	1.94	0.86
1:C:143:GLN:NE2	1:D:106:MET:CE	2.37	0.86
1:C:222:GLU:OE1	1:C:222:GLU:N	2.08	0.85
1:C:104:LEU:HD23	1:C:104:LEU:H	1.41	0.85
1:B:226:LYS:C	5:B:2100:HOH:O	2.16	0.83
1:D:195:ILE:O	1:D:199:THR:HG23	1.80	0.81
1:C:73:SER:H	1:C:76:GLN:NE2	1.79	0.80
1:C:100:ARG:NH2	5:C:2100:HOH:O	2.15	0.80
1:C:143:GLN:NE2	1:D:106:MET:SD	2.54	0.80
4:A:1001:DER:O1P	5:A:2098:HOH:O	1.98	0.80
1:D:106:MET:HG2	5:D:2045:HOH:O	1.82	0.80
1:D:9:ILE:HD12	1:D:224:VAL:HG13	1.64	0.78
1:A:9:ILE:HD12	1:A:223:GLY:O	1.84	0.78
1:D:1:MET:N	5:D:2112:HOH:O	2.15	0.77
1:D:13:GLU:OE1	1:D:226:LYS:NZ	2.15	0.75
1:B:154:ILE:HG22	1:B:154:ILE:O	1.86	0.73
1:C:186:ARG:HD2	1:C:188:ASP:OD1	1.87	0.73
1:A:1:MET:O	1:A:2:ASN:HB3	1.88	0.72
1:C:143:GLN:NE2	1:D:106:MET:HE2	2.04	0.71
1:B:3:VAL:HG23	5:B:2101:HOH:O	1.91	0.70
1:A:220:THR:HB	5:A:2106:HOH:O	1.90	0.70
1:B:4:GLU:O	1:B:7:LYS:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASN:C	1:D:2:ASN:HD22	1.95	0.68
1:C:129:TYR:CD1	1:C:186:ARG:HB2	2.29	0.67
1:C:222:GLU:H	1:C:222:GLU:CD	1.98	0.67
1:B:175:ASN:HB2	5:B:2106:HOH:O	1.94	0.66
1:D:130:LEU:O	1:D:131:CYS:HB2	1.96	0.65
1:C:150:GLU:OE2	5:C:2097:HOH:O	2.15	0.65
1:B:3:VAL:CG2	5:B:2101:HOH:O	2.45	0.64
1:C:1:MET:SD	1:C:220:THR:O	2.56	0.63
1:D:106:MET:SD	5:D:2060:HOH:O	2.55	0.63
1:B:220:THR:HG22	1:B:224:VAL:HA	1.80	0.63
1:C:106:MET:CE	5:C:2058:HOH:O	2.46	0.62
1:A:9:ILE:CD1	1:A:223:GLY:O	2.48	0.62
1:B:220:THR:O	1:B:221:ARG:C	2.38	0.62
1:B:106:MET:CE	5:B:2052:HOH:O	2.48	0.61
1:B:37:LYS:NZ	5:B:2076:HOH:O	2.33	0.61
1:B:18:ILE:HG22	1:B:48:ILE:CD1	2.29	0.61
1:C:45:ARG:NH1	5:C:2095:HOH:O	2.34	0.61
1:C:91:ASP:HB3	1:C:130:LEU:HD13	1.83	0.61
1:C:61:LYS:HG3	1:C:71:ILE:HD13	1.82	0.60
1:A:143:GLN:CD	1:B:106:MET:SD	2.79	0.60
1:D:191:LEU:HD22	1:D:211:ASP:OD2	2.00	0.60
1:A:195:ILE:O	1:A:199:THR:HG23	2.01	0.60
1:A:73:SER:H	1:A:76:GLN:NE2	1.99	0.60
1:B:106:MET:HE3	5:B:2052:HOH:O	2.01	0.59
1:D:14:ALA:HB2	1:D:120:LEU:HD21	1.84	0.59
1:B:37:LYS:NZ	5:B:2058:HOH:O	2.30	0.59
1:B:91:ASP:HB3	1:B:130:LEU:HD13	1.84	0.59
1:B:154:ILE:O	1:B:154:ILE:CG2	2.51	0.59
1:B:220:THR:HG22	1:B:224:VAL:CA	2.33	0.59
1:C:220:THR:HG22	1:C:221:ARG:H	1.69	0.58
1:D:1:MET:HA	5:D:2069:HOH:O	2.03	0.58
1:D:73:SER:H	1:D:76:GLN:NE2	2.02	0.58
1:C:130:LEU:O	1:C:131:CYS:HB2	2.03	0.58
1:A:130:LEU:O	1:A:131:CYS:HB2	2.04	0.57
1:D:128:ASP:HB2	1:D:132:GLN:HE22	1.68	0.57
1:D:4:GLU:OE2	1:D:34:TYR:OH	2.18	0.57
1:C:211:ASP:HA	1:C:229:ARG:HH22	1.70	0.57
1:A:62:LEU:HD23	5:D:2086:HOH:O	2.05	0.57
1:B:145:TRP:CZ3	5:B:2068:HOH:O	2.58	0.57
1:A:121:VAL:HB	1:A:125:LYS:HG3	1.87	0.57
1:A:123:GLU:HG3	1:A:220:THR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HH11	1:A:229:ARG:HB3	1.70	0.56
1:D:91:ASP:HB3	1:D:130:LEU:HD13	1.87	0.55
1:C:21:ASP:OD1	1:C:50:ASP:OD2	2.24	0.55
1:A:204:ILE:HG23	1:B:204:ILE:CD1	2.36	0.55
1:B:135:PRO:O	1:B:137:PRO:HD3	2.05	0.55
1:C:220:THR:HG22	1:C:221:ARG:N	2.22	0.55
1:B:229:ARG:HD3	1:B:229:ARG:H	1.71	0.55
1:C:104:LEU:CD2	1:C:104:LEU:H	2.17	0.55
1:B:220:THR:HG23	1:B:223:GLY:H	1.72	0.54
1:A:91:ASP:HB3	1:A:130:LEU:HD13	1.88	0.54
1:A:106:MET:CE	1:B:143:GLN:NE2	2.70	0.54
1:C:105:THR:HG23	5:D:2061:HOH:O	2.05	0.54
1:B:42:LYS:HG3	1:B:47:GLU:HB2	1.90	0.54
1:C:19:GLU:HG3	5:C:2040:HOH:O	2.08	0.54
1:B:2:ASN:O	1:B:6:MET:HE3	2.07	0.54
1:A:62:LEU:CD2	5:D:2086:HOH:O	2.55	0.54
1:C:106:MET:HE3	5:C:2058:HOH:O	2.08	0.53
1:B:220:THR:CG2	1:B:224:VAL:N	2.72	0.53
1:C:106:MET:HE1	5:C:2058:HOH:O	2.07	0.53
1:B:130:LEU:O	1:B:131:CYS:HB2	2.08	0.53
5:C:2078:HOH:O	1:D:199:THR:HG22	2.08	0.52
1:B:58:TYR:O	1:B:62:LEU:HD23	2.10	0.52
1:D:91:ASP:HB2	1:D:92:PRO:CD	2.39	0.52
1:B:225:LYS:HG2	5:B:2100:HOH:O	2.08	0.52
1:B:104:LEU:H	1:B:104:LEU:HD23	1.74	0.52
1:B:224:VAL:HG22	1:B:225:LYS:N	2.25	0.51
1:B:4:GLU:O	1:B:7:LYS:HB2	2.11	0.51
1:D:131:CYS:O	1:D:183:LYS:HE3	2.11	0.51
1:A:13:GLU:CD	1:A:16:LYS:HD2	2.31	0.51
1:C:222:GLU:N	1:C:222:GLU:CD	2.60	0.51
1:A:13:GLU:OE1	1:A:16:LYS:HD2	2.11	0.51
1:C:129:TYR:CE1	1:C:186:ARG:HB2	2.44	0.50
1:D:129:TYR:CD1	1:D:186:ARG:HB2	2.46	0.50
1:D:49:SER:O	1:D:50:ASP:HB3	2.12	0.50
1:D:211:ASP:HA	1:D:229:ARG:HH12	1.76	0.50
1:D:6:MET:SD	1:D:123:GLU:HG3	2.52	0.50
1:D:97:ILE:HG13	1:D:130:LEU:HG	1.93	0.50
1:A:106:MET:HG2	5:A:2024:HOH:O	2.11	0.50
1:B:145:TRP:CH2	5:B:2068:HOH:O	2.54	0.50
1:C:88:ASP:O	5:C:2108:HOH:O	2.19	0.49
1:A:149:ILE:HG13	1:A:180:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ILE:HG23	1:B:204:ILE:HD12	1.94	0.49
1:C:1:MET:HG3	1:C:6:MET:HG3	1.95	0.49
1:B:225:LYS:C	5:B:2100:HOH:O	2.44	0.48
1:C:97:ILE:HG13	1:C:130:LEU:HG	1.95	0.48
2:D:2004:CL:CL	4:D:1004:DER:C1	2.93	0.48
1:B:2:ASN:C	1:B:2:ASN:OD1	2.52	0.48
1:A:6:MET:O	1:A:219:GLY:HA3	2.14	0.48
1:B:97:ILE:HG13	1:B:130:LEU:HG	1.95	0.48
1:B:220:THR:O	1:B:223:GLY:N	2.46	0.48
1:A:175:ASN:HB2	5:A:2048:HOH:O	2.14	0.47
1:B:18:ILE:HG22	1:B:48:ILE:HD11	1.93	0.47
1:B:41:GLU:HG2	5:B:2067:HOH:O	2.13	0.47
1:C:206:ASN:HD22	1:C:208:ILE:H	1.61	0.47
1:D:42:LYS:HA	1:D:45:ARG:HE	1.80	0.47
1:C:61:LYS:HE3	1:C:71:ILE:HD11	1.96	0.47
1:C:143:GLN:CD	1:D:106:MET:CE	2.83	0.47
1:B:94:LEU:HD22	1:B:216:VAL:HG21	1.95	0.47
1:B:220:THR:HG23	1:B:224:VAL:N	2.30	0.47
1:B:62:LEU:O	1:B:66:GLU:HG3	2.15	0.47
1:C:39:LEU:HD11	1:C:51:ILE:HD13	1.97	0.47
1:A:106:MET:HE2	1:B:143:GLN:NE2	2.30	0.47
1:D:148:ILE:O	1:D:152:LEU:HG	2.15	0.47
1:D:2:ASN:C	1:D:2:ASN:ND2	2.66	0.46
1:C:39:LEU:HD11	1:C:51:ILE:CD1	2.46	0.46
1:C:2:ASN:HB3	5:C:2070:HOH:O	2.15	0.46
1:C:143:GLN:CD	1:D:106:MET:HE1	2.36	0.46
1:B:73:SER:H	1:B:76:GLN:NE2	2.14	0.45
1:B:91:ASP:OD1	1:B:91:ASP:C	2.54	0.45
1:B:220:THR:CG2	1:B:224:VAL:CA	2.94	0.45
1:B:221:ARG:O	1:B:222:GLU:C	2.53	0.45
1:C:123:GLU:HG3	1:C:124:ARG:N	2.30	0.45
1:B:2:ASN:O	1:B:6:MET:CE	2.65	0.45
1:B:214:ASP:OD2	5:B:2069:HOH:O	2.21	0.45
1:A:1:MET:SD	1:A:220:THR:O	2.75	0.45
1:C:220:THR:HG22	1:C:222:GLU:OE1	2.17	0.45
1:C:220:THR:CG2	1:C:221:ARG:H	2.29	0.45
1:D:37:LYS:NZ	1:D:67:HIS:CE1	2.85	0.44
1:A:104:LEU:H	1:A:104:LEU:HD23	1.81	0.44
1:B:14:ALA:HB2	1:B:120:LEU:HD21	1.98	0.44
1:D:206:ASN:HD22	1:D:208:ILE:H	1.64	0.44
1:A:94:LEU:HD23	1:A:94:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HB2	1:B:184:PHE:CE2	2.52	0.44
1:C:19:GLU:C	1:C:48:ILE:HD11	2.38	0.44
1:A:215:ILE:HG12	1:A:228:GLU:OE2	2.18	0.43
1:B:106:MET:HE1	5:B:2052:HOH:O	2.14	0.43
1:B:224:VAL:HG22	1:B:225:LYS:H	1.83	0.43
1:B:37:LYS:HG2	1:B:67:HIS:CE1	2.54	0.43
1:A:5:GLU:O	1:A:9:ILE:HG23	2.18	0.43
1:B:127:VAL:HG12	1:B:133:LYS:HE3	2.00	0.43
1:A:148:ILE:O	1:A:152:LEU:HG	2.18	0.43
1:D:91:ASP:CB	1:D:92:PRO:CD	2.96	0.43
1:A:49:SER:O	1:A:50:ASP:HB3	2.19	0.43
1:D:104:LEU:H	1:D:104:LEU:HD23	1.84	0.43
1:D:24:ILE:HA	1:D:82:VAL:O	2.18	0.43
1:D:73:SER:H	1:D:76:GLN:HE21	1.66	0.42
1:B:145:TRP:CG	1:B:146:LYS:N	2.87	0.42
1:B:1:MET:SD	1:B:5:GLU:CB	3.07	0.42
1:C:94:LEU:HB2	1:C:229:ARG:HE	1.85	0.42
1:D:39:LEU:HD11	1:D:51:ILE:HD13	2.02	0.42
5:A:2084:HOH:O	1:D:62:LEU:HD21	2.20	0.42
1:C:220:THR:OG1	1:C:225:LYS:HD3	2.18	0.42
1:B:91:ASP:HB2	1:B:92:PRO:CD	2.50	0.41
1:B:133:LYS:NZ	5:B:2098:HOH:O	2.20	0.41
1:B:88:ASP:OD1	4:B:1002:DER:O3	2.30	0.41
1:C:2:ASN:ND2	1:C:3:VAL:H	2.19	0.41
1:D:2:ASN:ND2	1:D:5:GLU:H	2.19	0.41
1:C:9:ILE:HG13	5:C:2083:HOH:O	2.19	0.41
1:A:91:ASP:HB2	1:A:92:PRO:CD	2.51	0.41
1:A:87:ALA:HA	1:A:98:LYS:HG2	2.03	0.41
1:B:229:ARG:CD	1:B:229:ARG:H	2.33	0.40
1:B:195:ILE:O	1:B:199:THR:HG23	2.21	0.40
1:B:9:ILE:HD13	1:B:9:ILE:HA	1.87	0.40
1:C:100:ARG:NH1	4:C:1003:DER:O4	2.54	0.40
1:D:39:LEU:HD11	1:D:51:ILE:CD1	2.50	0.40
1:B:43:LEU:HD12	5:B:2102:HOH:O	2.21	0.40
1:C:21:ASP:HA	1:C:50:ASP:O	2.20	0.40
1:B:24:ILE:HA	1:B:82:VAL:O	2.22	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	227/229 (99%)	222 (98%)	4 (2%)	1 (0%)	34	30
1	B	227/229 (99%)	215 (95%)	9 (4%)	3 (1%)	12	6
1	C	227/229 (99%)	221 (97%)	5 (2%)	1 (0%)	34	30
1	D	227/229 (99%)	223 (98%)	4 (2%)	0	100	100
All	All	908/916 (99%)	881 (97%)	22 (2%)	5 (1%)	25	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	GLU
1	A	2	ASN
1	B	223	GLY
1	B	221	ARG
1	C	131	CYS

### 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	190/192 (99%)	184 (97%)	6 (3%)	39	38
1	B	190/192 (99%)	184 (97%)	6 (3%)	39	38
1	C	190/192 (99%)	184 (97%)	6 (3%)	39	38
1	D	190/192 (99%)	183 (96%)	7 (4%)	34	32
All	All	760/768 (99%)	735 (97%)	25 (3%)	38	37



All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	96	LEU
1	A	113	ARG
1	A	130	LEU
1	A	220	THR
1	A	229	ARG
1	B	96	LEU
1	B	130	LEU
1	B	131	CYS
1	B	220	THR
1	B	228	GLU
1	B	229	ARG
1	C	19	GLU
1	C	104	LEU
1	C	113	ARG
1	C	130	LEU
1	C	186	ARG
1	C	222	GLU
1	D	2	ASN
1	D	12	LYS
1	D	123	GLU
1	D	125	LYS
1	D	130	LEU
1	D	149	ILE
1	D	225	LYS

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

Mol	Chain	Res	Type
1	A	76	GLN
1	A	93	ASN
1	A	198	ASN
1	A	206	ASN
1	B	76	GLN
1	B	198	ASN
1	B	206	ASN
1	C	2	ASN
1	C	76	GLN
1	C	198	ASN
1	C	206	ASN
1	D	2	ASN

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Mol	Chain	Res	Type
1	D	67	HIS
1	D	76	GLN
1	D	93	ASN
1	D	132	GLN
1	D	198	ASN
1	D	206	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z  > 2$
4	DER	C	1003	-	9,12,12	0.76	0	12,17,17	1.16	1 (8%)
4	DER	B	1002	-	9,12,12	0.64	0	12,17,17	1.83	3 (25%)
4	DER	A	1001	-	9,12,12	0.63	0	12,17,17	1.02	1 (8%)
4	DER	D	1004	-	9,12,12	0.71	0	12,17,17	1.42	2 (16%)

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
4	DER	C	1003	-	-	0/10/14/14	-
4	DER	B	1002	-	-	6/10/14/14	-
4	DER	A	1001	-	-	0/10/14/14	-
4	DER	D	1004	-	-	2/10/14/14	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	DER	O4-C4-C3	-3.76	99.33	109.36
4	B	1002	DER	O3P-P-O2P	3.70	121.77	107.64
4	D	1004	DER	O3P-P-O4	-2.77	99.37	106.73
4	C	1003	DER	O3P-P-O2P	2.56	117.43	107.64
4	B	1002	DER	P-O4-C4	2.55	125.33	118.30
4	D	1004	DER	O3P-P-O2P	2.46	117.04	107.64
4	A	1001	DER	O3P-P-O2P	2.03	115.39	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	DER	C1-C2-C3-O3
4	B	1002	DER	C2-C3-C4-O4
4	B	1002	DER	O3-C3-C4-O4
4	D	1004	DER	C2-C3-C4-O4
4	B	1002	DER	C1-C2-C3-C4
4	B	1002	DER	O2-C2-C3-C4
4	D	1004	DER	O3-C3-C4-O4
4	B	1002	DER	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1003	DER	1	0
4	B	1002	DER	1	0
4	A	1001	DER	1	0
4	D	1004	DER	2	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	229/229 (100%)	0.24	12 (5%) 27 26	24, 39, 66, 79	0
1	B	229/229 (100%)	0.22	15 (6%) 18 17	23, 37, 62, 79	0
1	C	229/229 (100%)	0.16	13 (5%) 23 23	24, 37, 60, 76	0
1	D	229/229 (100%)	0.10	12 (5%) 27 26	23, 38, 59, 73	0
All	All	916/916 (100%)	0.18	52 (5%) 23 23	23, 37, 62, 79	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	6.3
1	B	223	GLY	5.1
1	B	1	MET	4.7
1	D	229	ARG	4.3
1	D	1	MET	4.2
1	D	188	ASP	4.2
1	A	229	ARG	4.1
1	B	229	ARG	4.0
1	A	44	LYS	3.9
1	A	222	GLU	3.9
1	A	223	GLY	3.8
1	D	222	GLU	3.8
1	B	221	ARG	3.8
1	A	1	MET	3.6
1	B	219	GLY	3.4
1	C	154	ILE	3.4
1	A	219	GLY	3.3
1	B	224	VAL	3.3
1	C	223	GLY	3.1
1	A	128	ASP	3.1
1	B	155	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	44	LYS	2.9
1	B	222	GLU	2.9
1	C	158	LYS	2.8
1	B	220	THR	2.8
1	C	2	ASN	2.8
1	D	156	ASN	2.7
1	C	221	ARG	2.7
1	B	130	LEU	2.6
1	B	188	ASP	2.6
1	D	189	ASP	2.6
1	B	92	PRO	2.6
1	C	78	ASP	2.5
1	D	211	ASP	2.5
1	D	39	LEU	2.5
1	C	128	ASP	2.4
1	C	222	GLU	2.4
1	A	47	GLU	2.4
1	D	158	LYS	2.3
1	A	221	ARG	2.3
1	A	123	GLU	2.3
1	D	154	ILE	2.3
1	C	44	LYS	2.2
1	A	127	VAL	2.2
1	B	189	ASP	2.2
1	C	224	VAL	2.1
1	C	219	GLY	2.1
1	B	50	ASP	2.1
1	D	185	PRO	2.1
1	B	129	TYR	2.1
1	C	220	THR	2.0
1	A	217	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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, 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
4	DER	A	1001	13/13	0.89	0.20	29,36,39,40	13
4	DER	B	1002	13/13	0.90	0.18	29,36,39,42	13
2	CL	C	2003	1/1	0.92	0.48	30,30,30,30	1
4	DER	C	1003	13/13	0.93	0.16	25,31,34,39	13
4	DER	D	1004	13/13	0.94	0.17	22,30,35,40	13
2	CL	B	2002	1/1	0.95	0.43	20,20,20,20	1
2	CL	D	2004	1/1	0.97	0.52	20,20,20,20	1
2	CL	A	2001	1/1	0.97	0.50	22,22,22,22	1
2	CL	C	2007	1/1	0.98	0.07	33,33,33,33	0
3	NA	A	2011	1/1	0.98	0.06	25,25,25,25	0
2	CL	B	2010	1/1	0.99	0.06	25,25,25,25	0
3	NA	C	2012	1/1	0.99	0.07	25,25,25,25	0
2	CL	A	2005	1/1	0.99	0.05	29,29,29,29	0
2	CL	A	2009	1/1	1.00	0.04	30,30,30,30	0
2	CL	D	2008	1/1	1.00	0.02	24,24,24,24	0
2	CL	B	2006	1/1	1.00	0.04	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.