



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:19 PM GMT

PDB ID : 1F0V  
Title : Crystal structure of an Rnase A dimer displaying a new type of 3D domain swapping  
Authors : Liu, Y.S.; Gotte, G.; Libonati, M.; Eisenberg, D.S.  
Deposited on : 2000-05-17  
Resolution : 1.70 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

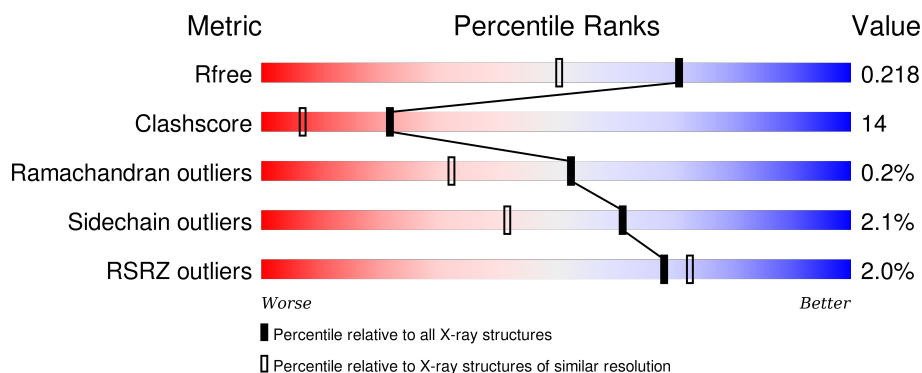
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	M	2	<div> <div>50%</div> <div>50%</div> </div>
1	N	2	<div> <div>100%</div> </div>
1	O	2	<div> <div>100%</div> </div>
1	P	2	<div> <div>100%</div> </div>
2	A	124	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	124	
2	C	124	
2	D	124	

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
3	PO4	A	801	-	-	X	-
4	GOL	A	908	-	-	-	X
4	GOL	A	915	-	-	-	X
4	GOL	A	918	-	-	X	X
4	GOL	B	902	-	X	X	-
4	GOL	B	905	-	-	X	X
4	GOL	B	907	-	-	-	X
4	GOL	B	910	-	-	X	X
4	GOL	B	914	-	-	-	X
4	GOL	B	920	-	-	X	-
4	GOL	B	921	-	-	-	X
4	GOL	B	922	-	-	X	-
4	GOL	C	903	-	-	-	X
4	GOL	C	917	-	-	X	X
4	GOL	D	901	-	X	X	X
4	GOL	D	913	-	X	X	-
4	GOL	D	916	-	-	-	X
4	GOL	D	924	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4742 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 DNA chain called 5'-D(\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
1	N	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
1	O	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			
1	P	2	Total	C	N	O	P	0	0	0
			38	19	8	10	1			

- Molecule 2 is a protein called RIBONUCLEASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	124	Total	C	N	O	S	0	4	0
			960	581	171	196	12			
2	B	124	Total	C	N	O	S	0	9	0
			979	594	174	198	13			
2	C	124	Total	C	N	O	S	0	6	0
			968	586	173	197	12			
2	D	124	Total	C	N	O	S	0	5	0
			965	585	172	196	12			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	154	Total	O		0	0
			154	154			
5	B	129	Total	O		0	0
			129	129			
5	C	132	Total	O		0	0
			132	132			
5	D	119	Total	O		0	0
			119	119			
5	M	3	Total	O		0	0
			3	3			
5	N	7	Total	O		0	0
			7	7			
5	O	3	Total	O		0	0
			3	3			
5	P	7	Total	O		0	0
			7	7			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-D(\*CP\*G)-3'



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There are no outlier residues recorded for this chain.

- Molecule 1: 5'-D(\*CP\*G)-3'



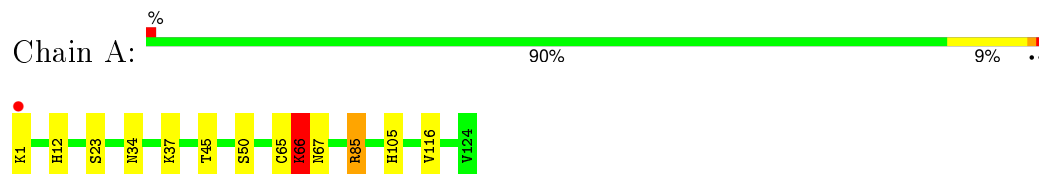
There are no outlier residues recorded for this chain.

- Molecule 1: 5'-D(\*CP\*G)-3'

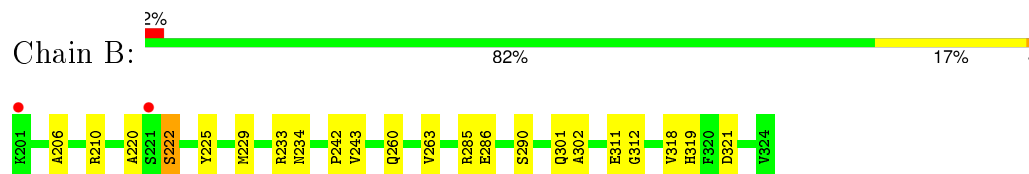


There are no outlier residues recorded for this chain.

- Molecule 2: RIBONUCLEASE A

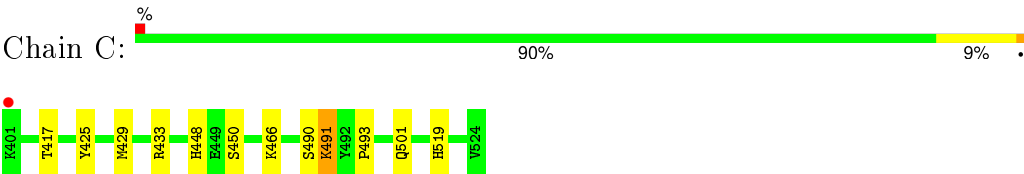


- Molecule 2: RIBONUCLEASE A

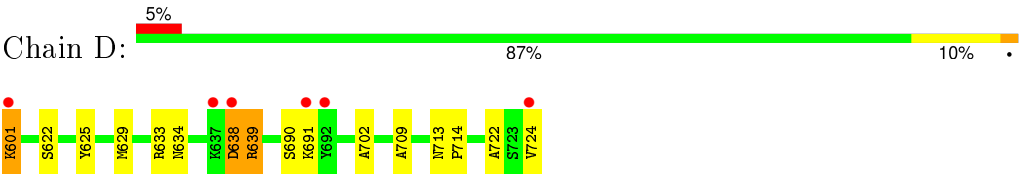


- Molecule 2: RIBONUCLEASE A





• Molecule 2: RIBONUCLEASE A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.57Å 96.34Å 48.24Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 15.72 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.0 (10.00-1.70) 95.1 (15.72-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.29 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.184 , 0.213 0.189 , 0.218	Depositor DCC
$R_{free}$ test set	7651 reflections (10.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 67.5	EDS
Estimated twinning fraction	0.002 for -h-l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 76031 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.85 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6604e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	M	1.11	0/42	1.08	0/63
1	N	1.29	0/42	1.14	0/63
1	O	1.28	0/42	1.03	0/63
1	P	1.44	0/42	1.05	0/63
2	A	0.91	1/992 (0.1%)	0.97	3/1335 (0.2%)
2	B	0.85	0/1032	0.90	0/1387
2	C	0.84	0/1009	0.90	1/1358 (0.1%)
2	D	0.88	0/1001	0.89	0/1346
All	All	0.89	1/4202 (0.0%)	0.92	4/5678 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	66	LYS	CE-NZ	5.03	1.61	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	85	ARG	NE-CZ-NH1	7.57	124.08	120.30
2	A	85	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	C	433	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	A	66	LYS	CD-CE-NZ	5.06	123.35	111.70

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	M	38	0	24	1	0
1	N	38	0	24	0	0
1	O	38	0	24	0	0
1	P	38	0	24	0	0
2	A	960	0	913	26	0
2	B	979	0	929	31	0
2	C	968	0	914	10	0
2	D	965	0	919	19	1
3	A	5	0	0	3	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	P	5	0	0	0	0
4	A	36	0	47	8	0
4	B	54	0	72	35	0
4	C	24	0	32	8	1
4	D	30	0	38	19	0
5	A	154	0	0	2	0
5	B	129	0	0	0	0
5	C	132	0	0	0	0
5	D	119	0	0	1	0
5	M	3	0	0	0	0
5	N	7	0	0	0	0
5	O	3	0	0	0	0
5	P	7	0	0	0	0
All	All	4742	0	3960	115	1

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 14.

All (115) 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)
4:D:924:GOL:C2	4:D:924:GOL:C1	1.80	1.58
4:C:903:GOL:C2	4:C:903:GOL:C1	1.76	1.54
4:A:923:GOL:C1	4:A:923:GOL:O1	1.65	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:910:GOL:O1	4:B:910:GOL:C1	1.65	1.43
4:B:902:GOL:C3	4:B:902:GOL:O3	1.66	1.43
4:D:901:GOL:C2	4:D:901:GOL:O2	1.67	1.43
4:B:920:GOL:O1	4:B:920:GOL:C1	1.67	1.42
4:A:918:GOL:O2	4:A:918:GOL:C2	1.66	1.42
4:B:905:GOL:C1	4:B:905:GOL:O1	1.70	1.40
4:B:920:GOL:C3	4:B:920:GOL:O3	1.67	1.40
4:D:913:GOL:O2	4:D:913:GOL:C2	1.69	1.39
4:B:914:GOL:C1	4:B:914:GOL:O1	1.66	1.39
4:C:917:GOL:O3	4:C:917:GOL:C3	1.69	1.39
4:A:911:GOL:C3	4:A:911:GOL:O3	1.71	1.38
4:D:913:GOL:O1	4:D:913:GOL:C1	1.70	1.37
4:D:901:GOL:C3	4:D:901:GOL:O3	1.76	1.32
4:B:921:GOL:C3	4:B:921:GOL:O3	1.81	1.26
4:D:924:GOL:O1	4:D:924:GOL:C1	1.83	1.25
2:A:66:LYS:HD3	2:A:67:ASN:H	1.19	1.02
2:B:301:GLN:HG3	4:B:906:GOL:H12	1.37	1.01
2:B:312:GLY:HA2	4:B:910:GOL:H31	1.44	0.97
2:B:210:ARG:HB2	4:B:905:GOL:H32	1.47	0.96
2:A:116:VAL:HG22	4:B:910:GOL:H12	1.51	0.91
2:C:450:SER:HB2	4:C:919:GOL:H32	1.68	0.76
2:A:66:LYS:HD3	2:A:67:ASN:N	2.01	0.75
2:D:714:PRO:O	4:D:901:GOL:H11	1.90	0.72
2:D:691[A]:LYS:NZ	2:D:691[A]:LYS:HB3	2.05	0.71
2:C:519[B]:HIS:HD2	2:D:709:ALA:HB2	1.56	0.70
2:C:501:GLN:HG3	4:C:917:GOL:H31	1.74	0.70
2:C:450:SER:CB	4:C:919:GOL:H32	2.23	0.69
2:C:490:SER:O	2:C:491:LYS:HD3	1.94	0.67
2:A:116:VAL:CG2	4:B:910:GOL:H12	2.23	0.67
2:A:34:ASN:HB3	2:A:37:LYS:HZ2	1.59	0.67
2:A:12:HIS:HE1	3:A:801:PO4:O2	1.77	0.66
2:C:519[B]:HIS:HD2	2:D:709:ALA:CB	2.08	0.66
2:B:302:ALA:HA	4:B:902:GOL:H32	1.78	0.65
2:A:12:HIS:HD2	2:A:45:THR:O	1.79	0.65
2:B:234:ASN:HD22	4:B:922:GOL:H32	1.61	0.64
4:D:913:GOL:O2	4:D:913:GOL:H2	1.92	0.63
2:D:702:ALA:HA	4:D:913:GOL:H2	1.79	0.62
2:B:220:ALA:O	2:B:301:GLN:NE2	2.29	0.62
2:B:234:ASN:ND2	4:B:922:GOL:H32	2.16	0.61
2:B:243:VAL:HG13	2:B:285:ARG:HE	1.66	0.60
2:C:466:LYS:HE2	2:D:722:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:GLN:HG3	4:C:917:GOL:C3	2.32	0.59
2:B:206:ALA:HB1	4:B:905:GOL:H12	1.83	0.59
2:D:639:ARG:HB3	2:D:639:ARG:HH11	1.67	0.59
2:B:242:PRO:HD2	4:B:914:GOL:H32	1.84	0.59
2:A:66:LYS:CD	2:A:67:ASN:H	2.04	0.59
4:B:910:GOL:HO1	4:B:910:GOL:C1	2.09	0.58
2:D:713:ASN:HB3	4:D:901:GOL:H12	1.84	0.58
2:A:34:ASN:HB3	2:A:37:LYS:NZ	2.17	0.58
4:C:917:GOL:HO3	4:C:917:GOL:C3	2.12	0.58
2:D:601:LYS:HD2	2:D:601:LYS:N	2.18	0.58
4:D:901:GOL:H12	5:D:1254:HOH:O	2.03	0.57
2:D:702:ALA:HA	4:D:913:GOL:H31	1.85	0.57
4:A:923:GOL:C1	4:A:923:GOL:HO1	2.08	0.56
4:D:913:GOL:HO2	4:D:913:GOL:C2	2.12	0.56
2:B:234:ASN:HD22	4:B:922:GOL:C3	2.19	0.55
2:A:105:HIS:HE1	5:A:1128:HOH:O	1.89	0.55
2:A:66:LYS:HD2	2:B:321:ASP:OD1	2.07	0.55
4:B:902:GOL:C3	4:B:902:GOL:HO3	2.10	0.55
2:A:65:CYS:HB3	2:A:66:LYS:CD	2.36	0.55
2:A:23:SER:HA	4:A:918:GOL:H11	1.89	0.55
2:B:210:ARG:CB	4:B:905:GOL:H32	2.31	0.54
4:D:913:GOL:HO1	4:D:913:GOL:C1	2.14	0.54
2:B:260:GLN:NE2	4:B:921:GOL:H2	2.23	0.53
2:A:66:LYS:HE2	5:A:1097:HOH:O	2.08	0.53
2:B:312:GLY:CA	4:B:910:GOL:H31	2.29	0.53
4:B:910:GOL:O3	4:B:920:GOL:H31	2.10	0.52
4:B:920:GOL:C3	4:B:920:GOL:HO3	2.11	0.52
2:D:638:ASP:HB3	2:D:639:ARG:HH12	1.75	0.51
2:A:66:LYS:N	2:A:66:LYS:CD	2.74	0.51
1:M:751:DC:C6	2:A:85:ARG:HD2	2.45	0.51
2:A:66:LYS:CD	2:B:321:ASP:OD1	2.59	0.50
2:B:285:ARG:HG3	2:B:285:ARG:HH11	1.77	0.50
2:B:225:TYR:CZ	2:B:229[A]:MET:HG3	2.46	0.50
4:B:914:GOL:HO1	4:B:914:GOL:C1	2.10	0.50
2:B:210:ARG:HB2	4:B:905:GOL:C3	2.30	0.50
4:D:901:GOL:HO2	4:D:901:GOL:C2	2.10	0.49
4:A:918:GOL:C2	4:A:918:GOL:HO2	2.10	0.49
2:D:625:TYR:CZ	2:D:629:MET:HG3	2.48	0.49
2:A:65:CYS:HB3	2:A:66:LYS:HD2	1.94	0.48
3:A:801:PO4:O1	2:B:319[A]:HIS:ND1	2.43	0.47
2:D:691[A]:LYS:HZ3	2:D:691[A]:LYS:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:12:HIS:CE1	3:A:801:PO4:O2	2.64	0.47
4:C:903:GOL:C3	4:C:903:GOL:C1	2.84	0.46
2:D:633:ARG:O	2:D:634:ASN:HB2	2.15	0.46
4:B:920:GOL:HO1	4:B:920:GOL:C1	2.11	0.46
4:B:905:GOL:C1	4:B:905:GOL:HO1	2.13	0.45
2:B:311:GLU:O	4:B:910:GOL:H2	2.17	0.45
2:B:302:ALA:HA	4:B:902:GOL:C3	2.45	0.45
2:B:229[B]:MET:HE3	2:B:233:ARG:CZ	2.46	0.45
2:A:66:LYS:HD2	2:A:66:LYS:H	1.82	0.44
2:B:286:GLU:HG3	2:B:290:SER:CB	2.47	0.44
2:D:702:ALA:HA	4:D:913:GOL:C2	2.44	0.44
2:D:702:ALA:CA	4:D:913:GOL:H31	2.47	0.44
2:A:66:LYS:CG	2:A:67:ASN:N	2.81	0.44
2:A:50:SER:OG	4:A:908:GOL:H31	2.18	0.44
2:B:206:ALA:O	4:B:905:GOL:H12	2.19	0.43
2:B:263:VAL:HB	4:B:907:GOL:H32	2.01	0.42
2:A:23:SER:HA	4:A:918:GOL:C1	2.50	0.42
4:D:924:GOL:C3	4:D:924:GOL:C1	2.86	0.42
2:D:702:ALA:HA	4:D:913:GOL:C3	2.48	0.42
2:A:66:LYS:N	2:A:66:LYS:HD2	2.34	0.42
2:B:210:ARG:HD2	4:B:922:GOL:H31	2.01	0.41
2:A:66:LYS:CD	2:A:67:ASN:N	2.75	0.41
2:C:417:THR:O	2:C:448:HIS:HB3	2.21	0.41
2:B:210:ARG:CD	4:B:922:GOL:H31	2.50	0.41
2:A:66:LYS:HE3	2:B:319[A]:HIS:NE2	2.36	0.40
2:B:318:VAL:HG23	2:B:319[B]:HIS:CD2	2.55	0.40
2:B:225:TYR:CZ	2:B:229[B]:MET:HG3	2.57	0.40
2:C:425:TYR:CZ	2:C:429:MET:HG3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:690:SER:O	4:C:919:GOL:O3[2_555]	1.96	0.24

## 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	
2	A	125/124 (101%)	121 (97%)	4 (3%)	0	100	100
2	B	130/124 (105%)	123 (95%)	6 (5%)	1 (1%)	24	7
2	C	127/124 (102%)	122 (96%)	5 (4%)	0	100	100
2	D	126/124 (102%)	118 (94%)	8 (6%)	0	100	100
All	All	508/496 (102%)	484 (95%)	23 (4%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	222	SER

### 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	
2	A	113/109 (104%)	111 (98%)	2 (2%)	66	49
2	B	118/109 (108%)	117 (99%)	1 (1%)	86	79
2	C	115/109 (106%)	113 (98%)	2 (2%)	68	51
2	D	114/109 (105%)	110 (96%)	4 (4%)	43	20
All	All	460/436 (106%)	451 (98%)	9 (2%)	61	44

All (9) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	A	1	LYS
2	A	66	LYS
2	B	222	SER
2	C	491	LYS
2	C	493	PRO
2	D	601	LYS
2	D	622	SER
2	D	638	ASP
2	D	639	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	11	GLN
2	A	12	HIS
2	A	105	HIS
2	B	228	GLN
2	B	234	ASN
2	C	434	ASN
2	C	503	ASN
2	C	505	HIS
2	D	634	ASN
2	D	674	GLN

### 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](#)

28 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	PO4	A	801	-	4,4,4	0.83	0	6,6,6	0.28	0
4	GOL	A	904	-	5,5,5	3.52	5 (100%)	5,5,5	0.96	0
4	GOL	A	908	-	5,5,5	2.63	4 (80%)	5,5,5	0.66	0
4	GOL	A	911	-	5,5,5	3.78	2 (40%)	5,5,5	1.05	0
4	GOL	A	915	-	5,5,5	2.46	3 (60%)	5,5,5	0.81	0
4	GOL	A	918	-	5,5,5	4.09	3 (60%)	5,5,5	1.48	1 (20%)
4	GOL	A	923	-	5,5,5	4.02	3 (60%)	5,5,5	1.29	0
3	PO4	B	802	-	4,4,4	0.76	0	6,6,6	0.27	0
4	GOL	B	902	-	5,5,5	4.24	5 (100%)	5,5,5	1.62	1 (20%)
4	GOL	B	905	-	5,5,5	3.09	1 (20%)	5,5,5	1.91	2 (40%)
4	GOL	B	906	-	5,5,5	2.43	2 (40%)	5,5,5	0.70	0
4	GOL	B	907	-	5,5,5	1.92	3 (60%)	5,5,5	0.97	0
4	GOL	B	910	-	5,5,5	2.80	2 (40%)	5,5,5	2.06	2 (40%)
4	GOL	B	914	-	5,5,5	4.35	4 (80%)	5,5,5	1.50	1 (20%)
4	GOL	B	920	-	5,5,5	4.57	3 (60%)	5,5,5	0.83	0
4	GOL	B	921	-	5,5,5	4.39	3 (60%)	5,5,5	1.18	0
4	GOL	B	922	-	5,5,5	4.39	5 (100%)	5,5,5	0.73	0
3	PO4	C	803	-	4,4,4	0.69	0	6,6,6	0.28	0
4	GOL	C	903	-	5,5,5	3.48	2 (40%)	5,5,5	0.79	0
4	GOL	C	912	-	5,5,5	2.87	4 (80%)	5,5,5	0.79	0
4	GOL	C	917	-	5,5,5	3.12	2 (40%)	5,5,5	1.30	0
4	GOL	C	919	-	5,5,5	2.56	3 (60%)	5,5,5	1.38	1 (20%)
4	GOL	D	901	-	5,5,5	5.47	4 (80%)	5,5,5	2.29	3 (60%)
4	GOL	D	909	-	5,5,5	2.20	3 (60%)	5,5,5	0.86	0
4	GOL	D	913	-	5,5,5	5.46	4 (80%)	5,5,5	1.71	2 (40%)
4	GOL	D	916	-	5,5,5	2.56	3 (60%)	5,5,5	1.00	0
4	GOL	D	924	-	5,5,5	6.01	4 (80%)	5,5,5	0.62	0
3	PO4	P	804	-	4,4,4	0.95	0	6,6,6	0.28	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	PO4	A	801	-	-	0/0/0/0	0/0/0/0
4	GOL	A	904	-	-	0/4/4/4	0/0/0/0
4	GOL	A	908	-	-	0/4/4/4	0/0/0/0
4	GOL	A	911	-	-	0/4/4/4	0/0/0/0
4	GOL	A	915	-	-	0/4/4/4	0/0/0/0
4	GOL	A	918	-	-	0/4/4/4	0/0/0/0
4	GOL	A	923	-	-	0/4/4/4	0/0/0/0
3	PO4	B	802	-	-	0/0/0/0	0/0/0/0
4	GOL	B	902	-	-	0/4/4/4	0/0/0/0
4	GOL	B	905	-	-	0/4/4/4	0/0/0/0
4	GOL	B	906	-	-	0/4/4/4	0/0/0/0
4	GOL	B	907	-	-	0/4/4/4	0/0/0/0
4	GOL	B	910	-	-	0/4/4/4	0/0/0/0
4	GOL	B	914	-	-	0/4/4/4	0/0/0/0
4	GOL	B	920	-	-	0/4/4/4	0/0/0/0
4	GOL	B	921	-	-	0/4/4/4	0/0/0/0
4	GOL	B	922	-	-	0/4/4/4	0/0/0/0
3	PO4	C	803	-	-	0/0/0/0	0/0/0/0
4	GOL	C	903	-	-	0/4/4/4	0/0/0/0
4	GOL	C	912	-	-	0/4/4/4	0/0/0/0
4	GOL	C	917	-	-	0/4/4/4	0/0/0/0
4	GOL	C	919	-	-	0/4/4/4	0/0/0/0
4	GOL	D	901	-	-	0/4/4/4	0/0/0/0
4	GOL	D	909	-	-	0/4/4/4	0/0/0/0
4	GOL	D	913	-	-	0/4/4/4	0/0/0/0
4	GOL	D	916	-	-	0/4/4/4	0/0/0/0
4	GOL	D	924	-	-	0/4/4/4	0/0/0/0
3	PO4	P	804	-	-	0/0/0/0	0/0/0/0

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	913	GOL	O3-C3	-4.81	1.21	1.42
4	B	922	GOL	C3-C2	-2.56	1.42	1.52
4	C	919	GOL	O2-C2	-2.05	1.37	1.43
4	D	909	GOL	O3-C3	2.05	1.51	1.42
4	C	912	GOL	C3-C2	2.06	1.60	1.52
4	B	907	GOL	C3-C2	2.18	1.60	1.52
4	A	915	GOL	C1-C2	2.25	1.60	1.52
4	A	908	GOL	O2-C2	2.30	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	GOL	O1-C1	2.30	1.52	1.42
4	D	916	GOL	O1-C1	2.32	1.52	1.42
4	B	921	GOL	C1-C2	2.39	1.61	1.52
4	B	907	GOL	O3-C3	2.42	1.52	1.42
4	A	904	GOL	C3-C2	2.43	1.61	1.52
4	C	912	GOL	O3-C3	2.49	1.53	1.42
4	B	907	GOL	C1-C2	2.55	1.62	1.52
4	A	918	GOL	C3-C2	2.59	1.62	1.52
4	A	904	GOL	O3-C3	2.62	1.53	1.42
4	D	901	GOL	C1-C2	2.63	1.62	1.52
4	A	904	GOL	O2-C2	2.64	1.51	1.43
4	D	916	GOL	C1-C2	2.66	1.62	1.52
4	B	910	GOL	O3-C3	2.70	1.54	1.42
4	B	921	GOL	O1-C1	2.71	1.54	1.42
4	D	909	GOL	O2-C2	2.79	1.51	1.43
4	D	913	GOL	C1-C2	2.83	1.63	1.52
4	A	908	GOL	C3-C2	2.88	1.63	1.52
4	A	908	GOL	O1-C1	2.89	1.54	1.42
4	C	917	GOL	O1-C1	2.91	1.54	1.42
4	B	922	GOL	O3-C3	2.99	1.55	1.42
4	B	902	GOL	C3-C2	3.10	1.64	1.52
4	D	909	GOL	C3-C2	3.11	1.64	1.52
4	A	915	GOL	O3-C3	3.17	1.56	1.42
4	B	902	GOL	C1-C2	3.17	1.64	1.52
4	C	919	GOL	C1-C2	3.34	1.65	1.52
4	B	906	GOL	O2-C2	3.47	1.53	1.43
4	A	915	GOL	C3-C2	3.49	1.65	1.52
4	A	908	GOL	C1-C2	3.53	1.65	1.52
4	D	924	GOL	O2-C2	3.56	1.54	1.43
4	C	912	GOL	O1-C1	3.58	1.57	1.42
4	C	919	GOL	O1-C1	3.69	1.58	1.42
4	A	918	GOL	O3-C3	3.74	1.58	1.42
4	B	906	GOL	O3-C3	3.83	1.58	1.42
4	D	901	GOL	O1-C1	3.91	1.59	1.42
4	C	903	GOL	O3-C3	4.10	1.60	1.42
4	B	914	GOL	C3-C2	4.10	1.68	1.52
4	B	914	GOL	O3-C3	4.11	1.60	1.42
4	A	911	GOL	C3-C2	4.14	1.68	1.52
4	A	923	GOL	C1-C2	4.14	1.68	1.52
4	C	912	GOL	C1-C2	4.19	1.68	1.52
4	D	924	GOL	O3-C3	4.35	1.61	1.42
4	D	916	GOL	O3-C3	4.36	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	GOL	C1-C2	4.45	1.69	1.52
4	B	922	GOL	O1-C1	4.69	1.62	1.42
4	A	904	GOL	O1-C1	4.72	1.62	1.42
4	B	922	GOL	C1-C2	5.11	1.71	1.52
4	A	923	GOL	O1-C1	5.27	1.65	1.42
4	B	914	GOL	C1-C2	5.31	1.72	1.52
4	B	910	GOL	O1-C1	5.43	1.65	1.42
4	B	914	GOL	O1-C1	5.61	1.66	1.42
4	B	920	GOL	C1-C2	5.65	1.73	1.52
4	B	902	GOL	O3-C3	5.69	1.66	1.42
4	B	902	GOL	O2-C2	5.71	1.60	1.43
4	B	922	GOL	O2-C2	5.74	1.60	1.43
4	A	923	GOL	O2-C2	5.74	1.60	1.43
4	B	920	GOL	O3-C3	5.82	1.67	1.42
4	B	920	GOL	O1-C1	5.87	1.67	1.42
4	C	917	GOL	O3-C3	6.20	1.69	1.42
4	C	903	GOL	C1-C2	6.22	1.76	1.52
4	B	905	GOL	O1-C1	6.42	1.70	1.42
4	D	913	GOL	O1-C1	6.61	1.70	1.42
4	A	911	GOL	O3-C3	6.83	1.71	1.42
4	D	924	GOL	C1-C2	7.34	1.80	1.52
4	A	918	GOL	O2-C2	7.79	1.66	1.43
4	D	901	GOL	O3-C3	7.79	1.76	1.42
4	D	901	GOL	O2-C2	7.95	1.67	1.43
4	D	913	GOL	O2-C2	8.61	1.69	1.43
4	B	921	GOL	O3-C3	8.96	1.81	1.42
4	D	924	GOL	O1-C1	9.55	1.83	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	910	GOL	O2-C2-C3	-2.12	98.91	108.65
4	C	919	GOL	C3-C2-C1	-2.10	102.89	111.12
4	D	913	GOL	O2-C2-C3	2.09	118.24	108.65
4	D	901	GOL	C3-C2-C1	2.42	120.60	111.12
4	B	905	GOL	O2-C2-C1	2.43	119.80	108.65
4	B	914	GOL	O3-C3-C2	2.53	122.44	110.18
4	B	905	GOL	O1-C1-C2	2.71	123.34	110.18
4	D	901	GOL	O2-C2-C3	2.83	121.63	108.65
4	B	902	GOL	O2-C2-C3	2.88	121.83	108.65
4	D	913	GOL	O2-C2-C1	3.15	123.11	108.65
4	A	918	GOL	O2-C2-C3	3.27	123.65	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	GOL	O1-C1-C2	3.37	126.53	110.18
4	B	910	GOL	O1-C1-C2	3.99	129.51	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	PO4	3	0
4	A	908	GOL	1	0
4	A	911	GOL	1	0
4	A	918	GOL	4	0
4	A	923	GOL	2	0
4	B	902	GOL	4	0
4	B	905	GOL	7	0
4	B	906	GOL	1	0
4	B	907	GOL	1	0
4	B	910	GOL	8	0
4	B	914	GOL	3	0
4	B	920	GOL	5	0
4	B	921	GOL	2	0
4	B	922	GOL	5	0
4	C	903	GOL	2	0
4	C	917	GOL	4	0
4	C	919	GOL	2	1
4	D	901	GOL	6	0
4	D	913	GOL	10	0
4	D	924	GOL	3	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	M	2/2 (100%)	-0.76	0 100 100	17, 17, 17, 19	0
1	N	2/2 (100%)	-0.78	0 100 100	17, 17, 17, 18	0
1	O	2/2 (100%)	-0.80	0 100 100	18, 18, 18, 20	0
1	P	2/2 (100%)	-0.62	0 100 100	17, 17, 17, 18	0
2	A	124/124 (100%)	-0.23	1 (0%) 87 90	11, 17, 29, 49	0
2	B	124/124 (100%)	-0.11	2 (1%) 74 79	12, 17, 32, 49	0
2	C	124/124 (100%)	-0.16	1 (0%) 87 90	11, 18, 30, 47	0
2	D	124/124 (100%)	-0.05	6 (4%) 34 38	11, 18, 35, 48	0
All	All	504/504 (100%)	-0.15	10 (1%) 68 73	11, 18, 32, 49	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	601	LYS	5.4
2	B	201	LYS	5.3
2	C	401	LYS	4.6
2	A	1	LYS	4.5
2	B	221	SER	3.6
2	D	691[A]	LYS	2.8
2	D	637	LYS	2.5
2	D	724[A]	VAL	2.4
2	D	638	ASP	2.3
2	D	692	TYR	2.2

### 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 ⓘ

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
4	GOL	D	924	6/6	0.70	0.28	35.40	30,42,47,51	0
4	GOL	C	903	6/6	0.50	0.37	26.96	46,52,53,54	0
4	GOL	B	921	6/6	0.85	0.28	22.53	23,40,42,43	0
4	GOL	A	918	6/6	0.42	0.35	14.25	39,51,53,54	0
4	GOL	D	901	6/6	0.86	0.22	10.33	28,37,39,42	0
4	GOL	B	907	6/6	0.79	0.25	7.58	34,42,44,48	0
4	GOL	C	917	6/6	0.84	0.23	6.47	37,49,51,57	0
4	GOL	A	915	6/6	0.67	0.28	5.51	44,51,53,53	0
4	GOL	B	910	6/6	0.93	0.18	5.20	15,37,44,45	0
4	GOL	D	916	6/6	0.87	0.18	4.60	31,46,48,54	0
4	GOL	B	905	6/6	0.92	0.21	4.04	27,34,36,38	0
4	GOL	B	914	6/6	0.81	0.26	3.39	36,43,45,50	0
4	GOL	A	908	6/6	0.61	0.25	2.97	38,46,50,57	0
4	GOL	C	919	6/6	0.80	0.28	1.07	37,43,44,46	0
3	PO4	P	804	5/5	0.99	0.05	-1.52	14,14,22,22	0
3	PO4	A	801	5/5	0.99	0.05	-2.01	13,14,19,24	0
3	PO4	B	802	5/5	0.99	0.04	-2.01	12,14,21,22	0
3	PO4	C	803	5/5	0.99	0.04	-2.19	14,15,19,24	0
4	GOL	B	902	6/6	0.61	0.37	-	36,47,52,55	0
4	GOL	A	923	6/6	0.76	0.24	-	40,45,47,53	0
4	GOL	A	904	6/6	0.75	0.31	-	40,50,52,58	0
4	GOL	D	913	6/6	0.79	0.39	-	40,45,48,48	0
4	GOL	B	920	6/6	0.68	0.30	-	37,42,44,45	0
4	GOL	A	911	6/6	0.70	0.33	-	44,52,55,56	0
4	GOL	D	909	6/6	0.44	0.37	-	49,55,56,59	0
4	GOL	B	922	6/6	0.83	0.27	-	49,51,54,57	0
4	GOL	B	906	6/6	0.82	0.25	-	28,42,45,51	0
4	GOL	C	912	6/6	0.66	0.36	-	51,56,59,64	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.