



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WWG
Title : Plasmodium falciparum thymidylate kinase in complex with dGMP and ADP
Authors : Whittingham, J.L.; Carrero-Lerida, J.; Brannigan, J.A.; Ruiz-Perez, L.M.; Silva, A.P.; Fogg, M.J.; Wilkinson, A.J.; Gilbert, I.H.; Wilson, K.S.; Gonzalez-Pacanowska, D.
Deposited on : 2009-10-23
Resolution : 2.40 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

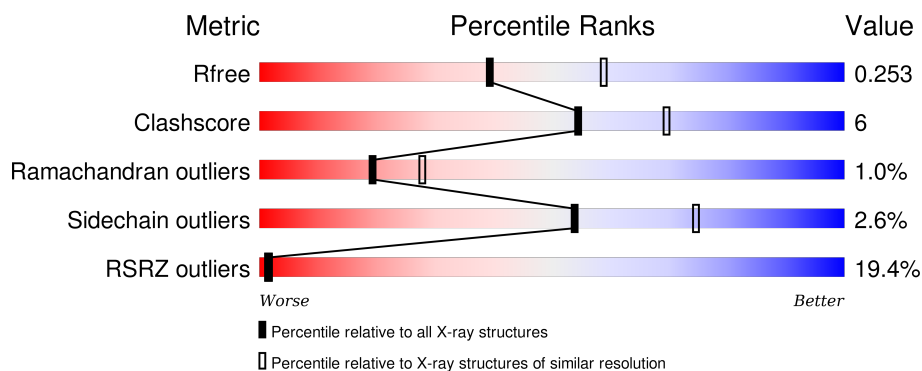
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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	212	 12% 80% 18% ..
1	B	212	 23% 81% 17% ..
1	C	212	 23% 80% 17% ..

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	DGP	C	211	-	-	-	X
5	GOL	A	1001	-	-	-	X
5	GOL	A	1002	-	-	-	X
5	GOL	A	1005	-	-	-	X
5	GOL	A	1007	-	-	-	X
5	GOL	B	1001	-	-	-	X
5	GOL	B	1002	-	-	-	X
5	GOL	B	1003	-	-	-	X
5	GOL	B	1004	-	-	-	X
5	GOL	B	1006	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5654 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.

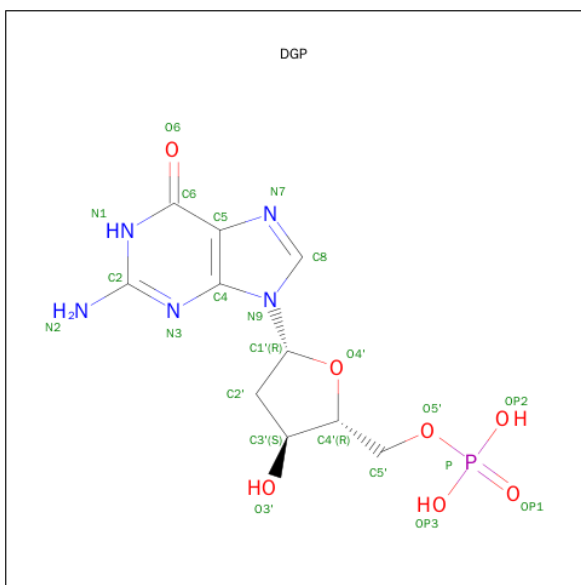
- Molecule 1 is a protein called THYMIDILATE KINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	14	0	0
			1735	1114	288	327	6			
1	B	210	Total	C	N	O	S	12	1	0
			1750	1124	291	328	7			
1	C	210	Total	C	N	O	S	23	0	0
			1743	1119	289	328	7			

There are 6 discrepancies between the modelled and reference sequences:

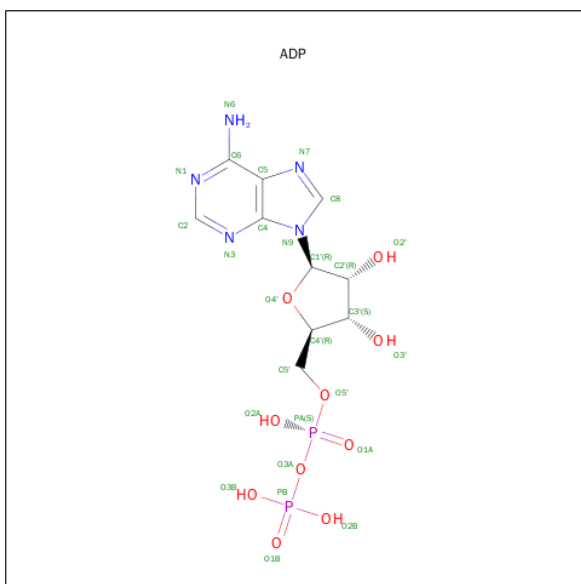
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q8I4S1
A	0	HIS	-	EXPRESSION TAG	UNP Q8I4S1
B	-1	SER	-	EXPRESSION TAG	UNP Q8I4S1
B	0	HIS	-	EXPRESSION TAG	UNP Q8I4S1
C	-1	SER	-	EXPRESSION TAG	UNP Q8I4S1
C	0	HIS	-	EXPRESSION TAG	UNP Q8I4S1

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (three-letter code: DGP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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

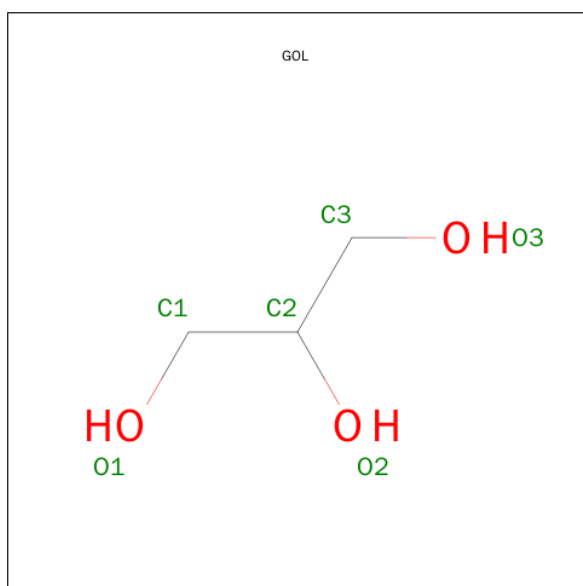


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

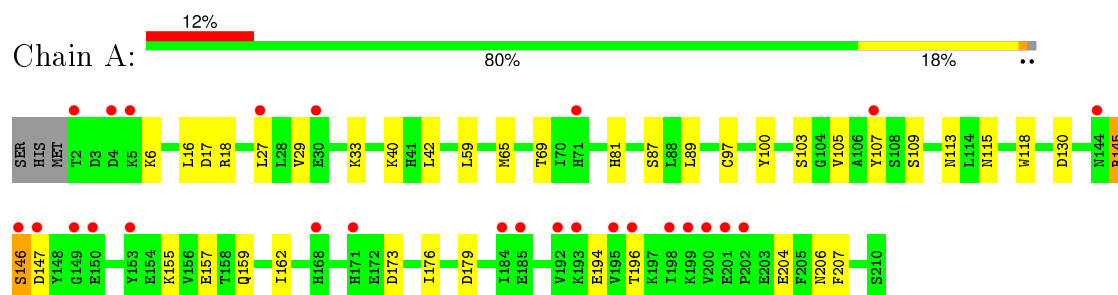
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		
6	B	64	Total	O	0	0
			64	64		
6	C	31	Total	O	0	0
			31	31		

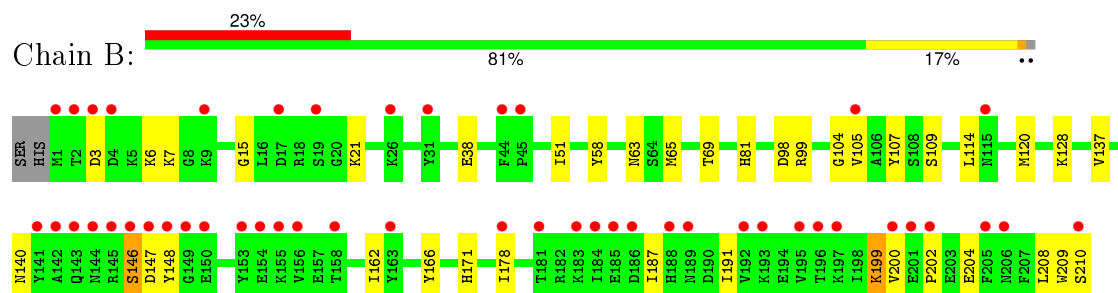
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

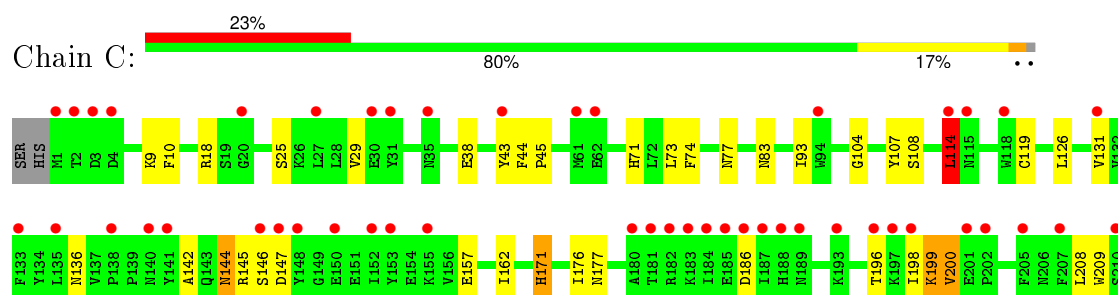
- Molecule 1: THYMIDILATE KINASE, PUTATIVE



- Molecule 1: THYMIDILATE KINASE, PUTATIVE



- Molecule 1: THYMIDILATE KINASE, PUTATIVE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.74Å 110.74Å 119.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.90 – 2.40 34.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (95.90-2.40) 99.2 (34.68-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.75 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.258 0.249 , 0.253	Depositor DCC
R_{free} test set	869 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.9	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 17222 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, DGP, ADP, NA

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	1.04	2/1777 (0.1%)	0.92	4/2399 (0.2%)
1	B	0.96	2/1796 (0.1%)	0.85	1/2424 (0.0%)
1	C	0.97	2/1785 (0.1%)	0.87	2/2409 (0.1%)
All	All	0.99	6/5358 (0.1%)	0.88	7/7232 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	LYS	CA-CB	-9.88	1.32	1.53
1	B	200	VAL	CA-CB	9.62	1.75	1.54
1	C	157	GLU	CB-CG	-6.23	1.40	1.52
1	C	209	TRP	CB-CG	-5.66	1.40	1.50
1	A	207	PHE	CE1-CZ	5.44	1.47	1.37
1	A	157	GLU	CB-CG	5.22	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	VAL	CB-CA-C	-7.42	97.31	111.40
1	A	204	GLU	CA-CB-CG	-6.97	98.06	113.40
1	C	171	HIS	CB-CA-C	6.87	124.14	110.40
1	A	155	LYS	CG-CD-CE	5.92	129.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	114	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	173	ASP	CB-CG-OD2	-5.34	113.49	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	171	HIS	CA

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	1735	0	1702	21	0
1	B	1750	0	1721	25	0
1	C	1743	0	1715	23	0
2	A	23	0	12	2	0
2	B	23	0	12	1	0
2	C	23	0	12	2	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	48	0	64	2	0
5	B	36	0	48	2	0
5	C	6	0	8	1	0
6	A	85	0	0	1	0
6	B	64	0	0	1	0
6	C	31	0	0	0	0
All	All	5654	0	5330	68	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 6.

All (68) 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:65:MET:CE	1:B:69:THR:HG22	2.18	0.73
1:C:199:LYS:O	1:C:200:VAL:HB	1.98	0.64
1:B:65:MET:HE2	1:B:69:THR:HG22	1.79	0.64
1:A:115:ASN:HD22	1:A:118:TRP:H	1.46	0.64
1:A:18:ARG:HH21	1:A:147:ASP:HB2	1.67	0.60
1:C:114:LEU:HD22	5:C:1001:GOL:H12	1.84	0.59
1:A:65:MET:CE	1:A:69:THR:HG22	2.34	0.57
1:B:65:MET:CE	1:B:69:THR:CG2	2.83	0.56
1:C:146:SER:O	1:C:147:ASP:HB2	2.06	0.55
1:C:131:VAL:HG21	1:C:176:ILE:HD12	1.89	0.55
1:B:81:HIS:CD2	5:B:1006:GOL:H32	2.43	0.54
1:C:107:TYR:CE1	2:C:211:DGP:H2'	2.43	0.54
1:A:176:ILE:HD13	1:A:194:GLU:HG2	1.90	0.53
1:B:137:VAL:O	1:B:137:VAL:HG13	2.09	0.52
1:B:105:VAL:O	1:B:109:SER:HB3	2.11	0.50
1:B:128:LYS:NZ	1:B:210:SER:O	2.35	0.49
1:A:16:LEU:HB3	1:A:159:GLN:NE2	2.28	0.49
1:C:136:ASN:HD22	1:C:177:ASN:HD21	1.59	0.49
1:A:107:TYR:CE1	2:A:211:DGP:H2'	2.48	0.49
1:A:145:ARG:O	1:A:146:SER:C	2.50	0.49
1:C:126:LEU:HB2	1:C:208:LEU:HD12	1.94	0.49
1:B:15:GLY:O	1:B:21:LYS:HE3	2.12	0.49
1:C:144:ASN:H	1:C:144:ASN:HD22	1.59	0.49
1:B:146:SER:C	1:B:148:TYR:H	2.16	0.48
1:A:6:LYS:HZ1	1:A:130:ASP:CG	2.16	0.48
1:C:43:TYR:N	1:C:43:TYR:CD1	2.81	0.48
1:A:59:LEU:HD13	2:A:211:DGP:H5'	1.95	0.47
1:A:17:ASP:H	1:A:159:GLN:HE22	1.61	0.47
1:A:196:THR:HA	5:A:1006:GOL:H12	1.96	0.47
1:C:38:GLU:HB2	1:C:93:ILE:HA	1.96	0.46
1:B:65:MET:HE2	1:B:69:THR:CG2	2.43	0.46
1:B:6:LYS:O	1:B:202:PRO:HA	2.16	0.46
1:B:98:ASP:O	1:B:99:ARG:HB2	2.17	0.45
1:B:208:LEU:HA	1:B:209:TRP:HA	1.73	0.45
1:B:187:ILE:HG22	1:B:191:ILE:HD12	1.99	0.44
1:A:42:LEU:O	1:A:97:CYS:HA	2.18	0.44
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.79	0.44
1:C:142:ALA:HB1	1:C:145:ARG:HD2	1.99	0.44
1:A:107:TYR:CE1	1:A:162:ILE:HD13	2.51	0.44
1:C:107:TYR:CE1	1:C:162:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:O	1:A:103:SER:HB2	2.17	0.44
1:C:108:SER:O	1:C:114:LEU:HB2	2.18	0.43
1:A:40:LYS:NZ	6:A:2018:HOH:O	2.40	0.43
1:C:74:PHE:O	1:C:77:ASN:HB3	2.19	0.43
1:C:18:ARG:HA	3:C:212:ADP:O3B	2.17	0.43
1:A:105:VAL:O	1:A:109:SER:HB3	2.19	0.43
1:B:107:TYR:CE1	1:B:162:ILE:HD13	2.54	0.43
1:B:21:LYS:HE2	1:B:99:ARG:CZ	2.48	0.42
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.94	0.42
1:C:104:GLY:O	1:C:108:SER:HB2	2.19	0.42
1:B:140:ASN:ND2	6:B:2045:HOH:O	2.52	0.42
1:C:25:SER:O	1:C:29:VAL:HG23	2.19	0.42
1:B:51:ILE:HG12	1:C:73:LEU:HD21	2.02	0.42
1:B:58:TYR:HA	1:B:63:ASN:OD1	2.20	0.42
1:A:65:MET:HE3	1:A:69:THR:CG2	2.50	0.41
1:B:104:GLY:HA2	2:B:211:DGP:O6	2.19	0.41
1:B:178:ILE:HG21	1:B:187:ILE:HG23	2.01	0.41
1:C:44:PHE:HA	1:C:45:PRO:C	2.40	0.41
1:C:107:TYR:CD1	2:C:211:DGP:H2'	2.56	0.41
1:C:9:LYS:HA	1:C:9:LYS:HD2	1.83	0.41
1:A:81:HIS:CD2	5:A:1005:GOL:H32	2.56	0.41
1:B:105:VAL:CG2	1:B:120:MET:HG3	2.51	0.41
1:B:3:ASP:OD2	1:B:7:LYS:NZ	2.52	0.41
1:C:108:SER:HB3	1:C:114:LEU:HD13	2.03	0.40
1:A:29:VAL:HG12	1:A:33:LYS:HE2	2.02	0.40
1:C:71:HIS:CE1	1:C:119:CYS:HB3	2.56	0.40
1:B:171:HIS:H	1:B:171:HIS:CD2	2.38	0.40
1:B:38:GLU:OE1	5:B:1002:GOL:O2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	207/212 (98%)	197 (95%)	9 (4%)	1 (0%)	34	48
1	B	209/212 (99%)	196 (94%)	11 (5%)	2 (1%)	19	28
1	C	208/212 (98%)	193 (93%)	12 (6%)	3 (1%)	14	19
All	All	624/636 (98%)	586 (94%)	32 (5%)	6 (1%)	19	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	SER
1	C	199	LYS
1	C	200	VAL
1	A	146	SER
1	B	147	ASP
1	C	198	ILE

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	192/195 (98%)	188 (98%)	4 (2%)	61	80
1	B	194/195 (100%)	190 (98%)	4 (2%)	61	80
1	C	193/195 (99%)	186 (96%)	7 (4%)	42	63
All	All	579/585 (99%)	564 (97%)	15 (3%)	54	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	113	ASN
1	A	145	ARG
1	A	206	ASN
1	B	114	LEU
1	B	166	TYR
1	B	199	LYS

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Mol	Chain	Res	Type
1	B	204	GLU
1	C	10	PHE
1	C	83	ASN
1	C	114	LEU
1	C	144	ASN
1	C	171	HIS
1	C	186	ASP
1	C	196	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	41	HIS
1	A	115	ASN
1	A	159	GLN
1	A	206	ASN
1	B	41	HIS
1	B	77	ASN
1	B	159	GLN
1	C	77	ASN
1	C	113	ASN
1	C	144	ASN
1	C	177	ASN
1	C	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 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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
5	GOL	A	1001	-	5,5,5	0.61	0	5,5,5	0.74	0
5	GOL	A	1002	-	5,5,5	0.59	0	5,5,5	0.76	0
5	GOL	A	1003	-	5,5,5	0.33	0	5,5,5	0.49	0
5	GOL	A	1004	-	5,5,5	0.43	0	5,5,5	0.44	0
5	GOL	A	1005	-	5,5,5	0.26	0	5,5,5	0.79	0
5	GOL	A	1006	-	5,5,5	0.32	0	5,5,5	0.29	0
5	GOL	A	1007	-	5,5,5	0.45	0	5,5,5	0.11	0
5	GOL	A	1008	-	5,5,5	0.35	0	5,5,5	0.49	0
2	DGP	A	211	4	21,25,25	1.75	6 (28%)	26,38,38	2.52	10 (38%)
3	ADP	A	212	4	22,29,29	1.56	4 (18%)	27,45,45	2.29	5 (18%)
5	GOL	B	1001	-	5,5,5	0.44	0	5,5,5	0.43	0
5	GOL	B	1002	-	5,5,5	0.70	0	5,5,5	0.71	0
5	GOL	B	1003	-	5,5,5	0.51	0	5,5,5	1.29	1 (20%)
5	GOL	B	1004	-	5,5,5	0.59	0	5,5,5	0.43	0
5	GOL	B	1005	-	5,5,5	0.36	0	5,5,5	0.48	0
5	GOL	B	1006	-	5,5,5	0.37	0	5,5,5	0.89	0
2	DGP	B	211	4	21,25,25	1.65	3 (14%)	26,38,38	1.76	7 (26%)
3	ADP	B	212	4	22,29,29	1.49	3 (13%)	27,45,45	2.63	7 (25%)
5	GOL	C	1001	-	5,5,5	0.27	0	5,5,5	0.41	0
2	DGP	C	211	4	21,25,25	2.25	4 (19%)	26,38,38	1.96	8 (30%)
3	ADP	C	212	4	22,29,29	2.15	3 (13%)	27,45,45	2.41	7 (25%)

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
5	GOL	A	1001	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1002	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1007	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1008	-	-	0/4/4/4	0/0/0/0
2	DGP	A	211	4	-	0/6/22/22	0/3/3/3
3	ADP	A	212	4	-	0/12/32/32	0/3/3/3
5	GOL	B	1001	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1002	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1003	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1004	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1005	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1006	-	-	0/4/4/4	0/0/0/0
2	DGP	B	211	4	-	0/6/22/22	0/3/3/3
3	ADP	B	212	4	-	0/12/32/32	0/3/3/3
5	GOL	C	1001	-	-	0/4/4/4	0/0/0/0
2	DGP	C	211	4	-	0/6/22/22	0/3/3/3
3	ADP	C	212	4	-	0/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	211	DGP	O5'-C5'	-3.85	1.29	1.44
3	A	212	ADP	PB-O3B	-2.86	1.44	1.54
2	A	211	DGP	P-OP3	-2.81	1.44	1.54
2	A	211	DGP	C6-N1	2.22	1.37	1.33
3	C	212	ADP	C5'-C4'	2.27	1.59	1.51
2	A	211	DGP	P-OP1	2.37	1.59	1.51
3	A	212	ADP	O4'-C4'	2.52	1.50	1.45
2	B	211	DGP	O4'-C1'	2.61	1.48	1.42
3	A	212	ADP	PA-O1A	2.64	1.60	1.51
2	A	211	DGP	P-O5'	2.92	1.70	1.60
3	B	212	ADP	PB-O1B	2.92	1.60	1.51
2	C	211	DGP	P-OP2	3.08	1.65	1.54
2	B	211	DGP	C6-N1	3.54	1.39	1.33
2	C	211	DGP	C6-N1	3.60	1.39	1.33
2	A	211	DGP	C2-N1	3.64	1.41	1.35
3	B	212	ADP	PA-O1A	3.64	1.64	1.51
3	A	212	ADP	O4'-C1'	3.85	1.46	1.41
3	B	212	ADP	O4'-C1'	3.90	1.46	1.41
2	B	211	DGP	C2-N1	4.94	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	211	DGP	C2-N1	5.05	1.44	1.35
3	C	212	ADP	O4'-C1'	6.13	1.49	1.41
2	C	211	DGP	P-OP1	6.26	1.71	1.51
3	C	212	ADP	PB-O1B	6.61	1.72	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	212	ADP	N3-C2-N1	-11.18	120.33	128.89
3	A	212	ADP	N3-C2-N1	-10.07	121.19	128.89
3	C	212	ADP	N3-C2-N1	-9.53	121.59	128.89
2	C	211	DGP	N3-C2-N1	-5.53	119.02	127.44
2	A	211	DGP	N3-C2-N1	-5.07	119.72	127.44
3	C	212	ADP	PA-O3A-PB	-4.84	116.44	132.67
2	B	211	DGP	N3-C2-N1	-4.07	121.24	127.44
2	A	211	DGP	C5-C6-N1	-3.80	118.40	123.59
3	B	212	ADP	PA-O3A-PB	-3.51	120.88	132.67
2	C	211	DGP	C1'-N9-C4	-3.27	121.61	127.16
2	B	211	DGP	C4-C5-N7	-3.26	106.48	109.48
2	A	211	DGP	C2'-C1'-N9	-3.20	106.38	114.16
2	A	211	DGP	OP2-P-OP1	-3.00	100.91	110.58
2	A	211	DGP	O3'-C3'-C4'	-2.86	98.50	110.05
2	B	211	DGP	C1'-N9-C4	-2.83	122.36	127.16
3	B	212	ADP	O2B-PB-O1B	-2.81	101.53	110.58
3	C	212	ADP	O5'-PA-O1A	-2.78	98.84	109.62
2	A	211	DGP	C4-C5-N7	-2.70	107.00	109.48
3	C	212	ADP	C4-C5-N7	-2.64	107.05	109.48
2	B	211	DGP	OP2-P-OP1	-2.53	102.45	110.58
2	C	211	DGP	C2'-C1'-N9	-2.52	108.03	114.16
3	B	212	ADP	C4-C5-N7	-2.41	107.26	109.48
2	C	211	DGP	C5-C6-N1	-2.38	120.33	123.59
3	B	212	ADP	C2'-C1'-N9	-2.37	110.68	114.29
2	A	211	DGP	OP2-P-O5'	-2.35	99.80	106.56
3	A	212	ADP	C1'-N9-C4	-2.31	123.46	126.94
3	C	212	ADP	O4'-C1'-N9	-2.24	103.41	108.10
2	A	211	DGP	C4'-O4'-C1'	-2.18	103.96	109.47
2	C	211	DGP	C4-C5-N7	-2.15	107.50	109.48
2	B	211	DGP	C5-C6-N1	-2.05	120.79	123.59
2	C	211	DGP	O5'-P-OP1	-2.02	101.99	107.14
3	A	212	ADP	O2B-PB-O1B	-2.01	104.10	110.58
2	B	211	DGP	O3'-C3'-C4'	-2.01	101.93	110.05
3	B	212	ADP	C2-N1-C6	2.01	122.36	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	212	ADP	C2-N1-C6	2.03	122.40	118.77
3	A	212	ADP	O2B-PB-O3A	2.08	114.53	105.09
5	B	1003	GOL	C3-C2-C1	2.22	119.83	111.12
3	C	212	ADP	O3A-PA-O5'	2.32	109.09	102.94
3	C	212	ADP	O2A-PA-O5'	2.39	120.51	108.46
3	B	212	ADP	O3B-PB-O3A	2.51	116.47	105.09
2	B	211	DGP	OP3-P-O5'	2.98	115.13	106.56
2	C	211	DGP	OP3-P-O5'	3.13	115.57	106.56
2	A	211	DGP	C6-N1-C2	3.25	120.44	115.94
2	C	211	DGP	N2-C2-N1	3.36	122.77	117.20
2	A	211	DGP	OP3-P-O5'	6.50	125.28	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	GOL	1	0
5	A	1006	GOL	1	0
2	A	211	DGP	2	0
5	B	1002	GOL	1	0
5	B	1006	GOL	1	0
2	B	211	DGP	1	0
5	C	1001	GOL	1	0
2	C	211	DGP	2	0
3	C	212	ADP	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, 95th 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 ²)	Q<0.9
1	A	209/212 (98%)	0.93	26 (12%) 5 5	21, 35, 59, 74	4 (1%)
1	B	210/212 (99%)	1.37	48 (22%) 1 1	25, 40, 69, 81	3 (1%)
1	C	210/212 (99%)	1.31	48 (22%) 1 1	29, 47, 68, 75	5 (2%)
All	All	629/636 (98%)	1.21	122 (19%) 1 1	21, 41, 67, 81	12 (1%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ASP	7.2
1	C	2	THR	6.4
1	B	184	ILE	5.8
1	C	184	ILE	5.4
1	C	180	ALA	5.3
1	C	27	LEU	4.9
1	B	141	TYR	4.7
1	C	189	ASN	4.7
1	B	148	TYR	4.6
1	A	2	THR	4.6
1	B	146	SER	4.5
1	B	192	VAL	4.5
1	A	147	ASP	4.4
1	B	202	PRO	4.4
1	A	198	ILE	4.3
1	C	187	ILE	4.3
1	C	3	ASP	4.2
1	B	150	GLU	4.1
1	A	200	VAL	4.1
1	B	2	THR	4.1
1	C	1	MET	4.0
1	C	31	TYR	4.0
1	B	183	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	144	ASN	3.7
1	C	188	HIS	3.6
1	B	1	MET	3.6
1	C	141	TYR	3.6
1	C	183	LYS	3.6
1	C	185	GLU	3.6
1	C	181	THR	3.5
1	B	158	THR	3.5
1	B	156	VAL	3.4
1	B	181	THR	3.4
1	C	198	ILE	3.4
1	B	149	GLY	3.4
1	B	189	ASN	3.3
1	A	202	PRO	3.3
1	C	210	SER	3.3
1	C	150	GLU	3.2
1	B	3	ASP	3.1
1	A	196	THR	3.1
1	B	210	SER	3.1
1	C	114	LEU	3.1
1	B	143	GLN	3.1
1	B	188	HIS	3.1
1	C	186	ASP	3.1
1	B	154	GLU	3.1
1	B	31	TYR	3.1
1	B	193	LYS	3.1
1	C	196	THR	3.1
1	C	94	TRP	3.1
1	C	4	ASP	3.0
1	A	171	HIS	3.0
1	A	5	LYS	3.0
1	B	197	LYS	3.0
1	B	178	ILE	2.9
1	B	200	VAL	2.9
1	B	9	LYS	2.9
1	B	196	THR	2.9
1	C	182	ARG	2.9
1	A	184	ILE	2.9
1	A	144	ASN	2.8
1	C	138	PRO	2.8
1	A	195	VAL	2.8
1	B	105	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	35	ASN	2.7
1	B	186	ASP	2.7
1	C	205	PHE	2.7
1	A	192	VAL	2.7
1	A	30	GLU	2.7
1	B	185	GLU	2.7
1	C	201	GLU	2.7
1	B	205	PHE	2.7
1	A	149	GLY	2.6
1	C	153	TYR	2.6
1	C	115	ASN	2.6
1	B	155	LYS	2.5
1	C	148	TYR	2.5
1	C	193	LYS	2.5
1	B	206	ASN	2.5
1	B	195	VAL	2.5
1	A	199	LYS	2.5
1	B	17	ASP	2.5
1	B	115	ASN	2.5
1	C	146	SER	2.5
1	B	163	TYR	2.4
1	C	135	LEU	2.4
1	C	155	LYS	2.4
1	A	150	GLU	2.4
1	A	153	TYR	2.4
1	B	153	TYR	2.4
1	A	146	SER	2.4
1	C	43	TYR	2.3
1	B	4	ASP	2.3
1	A	193	LYS	2.3
1	A	4	ASP	2.3
1	C	197	LYS	2.3
1	A	201	GLU	2.3
1	B	45	PRO	2.3
1	C	62	GLU	2.3
1	B	145	ARG	2.2
1	B	26	LYS	2.2
1	C	147	ASP	2.2
1	B	142	ALA	2.2
1	A	71	HIS	2.2
1	B	44	PHE	2.2
1	C	140	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	207	PHE	2.2
1	C	30	GLU	2.1
1	B	19	SER	2.1
1	A	107	TYR	2.1
1	B	201	GLU	2.1
1	C	202	PRO	2.1
1	A	168	HIS	2.1
1	C	20	GLY	2.1
1	C	61	MET	2.1
1	C	118	TRP	2.1
1	A	27	LEU	2.1
1	C	131	VAL	2.1
1	A	185	GLU	2.1
1	C	133	PHE	2.1
1	C	152	ILE	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, 95th 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 ²)	Q<0.9
5	GOL	A	1002	6/6	0.88	0.38	11.60	32,45,49,52	0
5	GOL	A	1005	6/6	0.86	0.45	10.99	75,77,78,78	0
5	GOL	B	1006	6/6	0.83	0.33	8.15	65,71,73,75	0
5	GOL	B	1003	6/6	0.78	0.29	7.05	45,47,47,48	0
5	GOL	A	1001	6/6	0.74	0.38	6.53	36,43,45,46	0
5	GOL	B	1002	6/6	0.69	0.37	6.12	50,51,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DGP	C	211	23/23	0.74	0.36	4.54	43,48,50,53	0
5	GOL	B	1001	6/6	0.94	0.34	2.74	40,43,43,44	0
5	GOL	A	1007	6/6	0.62	0.50	2.67	93,94,95,95	0
5	GOL	B	1004	6/6	0.91	0.25	2.42	56,58,60,63	0
2	DGP	A	211	23/23	0.84	0.29	1.60	22,27,37,38	0
5	GOL	A	1006	6/6	0.58	0.37	1.08	79,80,81,81	0
2	DGP	B	211	23/23	0.86	0.28	0.73	28,31,39,44	0
5	GOL	C	1001	6/6	0.94	0.23	-0.37	47,49,50,52	0
3	ADP	C	212	27/27	0.87	0.26	-0.38	39,53,55,56	0
3	ADP	A	212	27/27	0.91	0.19	-0.48	28,36,40,42	0
3	ADP	B	212	27/27	0.84	0.23	-0.90	43,50,53,54	0
5	GOL	A	1008	6/6	0.69	0.52	-	84,87,89,90	0
5	GOL	B	1005	6/6	0.75	0.32	-	74,76,79,81	0
4	NA	B	214	1/1	0.73	0.28	-	66,66,66,66	0
5	GOL	A	1004	6/6	0.57	0.39	-	70,73,77,79	0
4	NA	A	214	1/1	0.85	0.21	-	59,59,59,59	0
4	NA	C	214	1/1	0.48	0.48	-	55,55,55,55	0
4	NA	A	213	1/1	0.85	0.23	-	46,46,46,46	0
5	GOL	A	1003	6/6	0.69	0.34	-	82,84,84,85	0
4	NA	B	213	1/1	0.16	0.23	-	47,47,47,47	0
4	NA	C	213	1/1	0.81	0.54	-	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.