Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:05 PM GMT

PDB ID	:	5CDN
Title	:	2.8A structure of etoposide with S.aureus DNA gyrase and DNA
Authors	:	Bax, B.D.; Srikannathasan, V.; Chan, P.F.
Deposited on	:	2015-07-04
Resolution	:	2.79 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

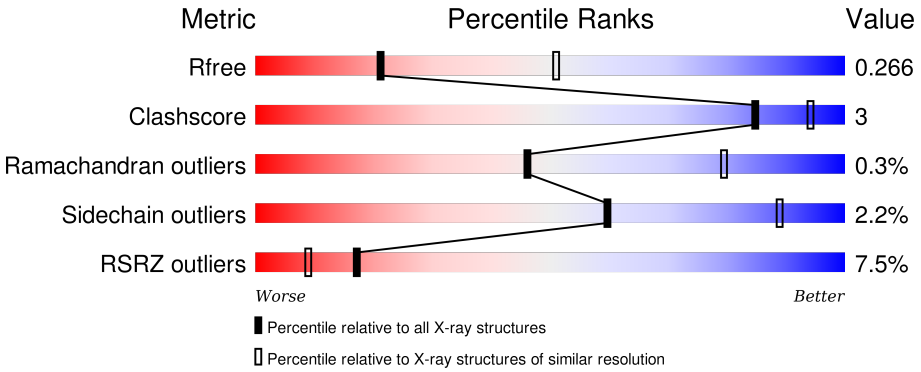
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	481	5% 91% 8%
1	C	481	3% 91% 8%
1	R	481	7% 90% 8%
1	T	481	9% 92% 7%
2	B	189	7% 86% 13%

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Mol	Chain	Length	Quality of chain
2	D	189	15% 85% 13%
2	S	189	10% 89% 11%
2	U	189	15% 88% 11%
3	E	8	100%
3	F	8	88% 13%
3	V	8	100%
3	W	8	88% 13%
4	G	12	75% 25%
4	N	12	50% 42% 8%
4	O	12	83% 17%
4	P	12	75% 25%

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
5	SO4	A	501	-	-	-	X
7	GOL	C	501	-	-	-	X
7	GOL	E	101	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23069 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	P	S	0	2	0
			3778	2348	682	731	1	16			
1	C	480	Total	C	N	O	P	S	0	0	0
			3775	2349	683	726	1	16			
1	R	475	Total	C	N	O	P	S	0	0	0
			3723	2320	670	716	1	16			
1	T	481	Total	C	N	O	P	S	0	5	0
			3798	2359	686	736	1	16			

- Molecule 2 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1456	912	251	284	9			
2	D	187	Total	C	N	O	S	0	1	0
			1433	898	250	276	9			
2	S	188	Total	C	N	O	S	0	0	0
			1437	903	249	276	9			
2	U	189	Total	C	N	O	S	0	1	0
			1447	908	255	275	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937
S	544	THR	-	linker	UNP P66937
S	545	GLY	-	linker	UNP P66937
U	544	THR	-	linker	UNP P66937
U	545	GLY	-	linker	UNP P66937

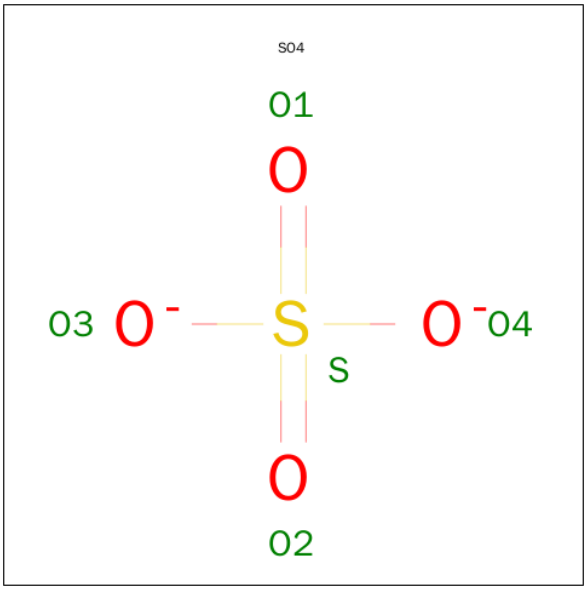
- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP**GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	P	0	0	0
			162	78	33	44	7			
3	F	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
3	V	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
3	W	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	12	Total	C	N	O	P	0	0	0
			240	115	44	70	11			
4	O	12	Total	C	N	O	P	0	0	0
			227	108	41	67	11			
4	N	12	Total	C	N	O	P	0	1	0
			259	124	47	76	12			
4	P	12	Total	C	N	O	P	0	0	0
			231	111	41	68	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

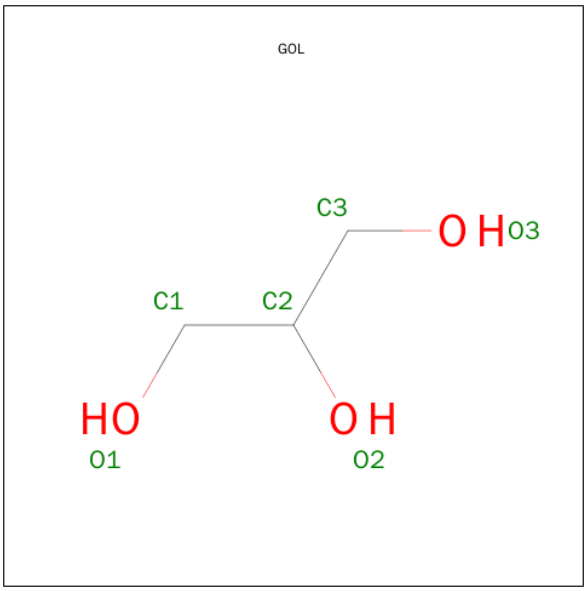


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mn 1 1	0	0
6	D	1	Total Mn 1 1	0	0
6	S	1	Total Mn 1 1	0	0
6	U	1	Total Mn 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

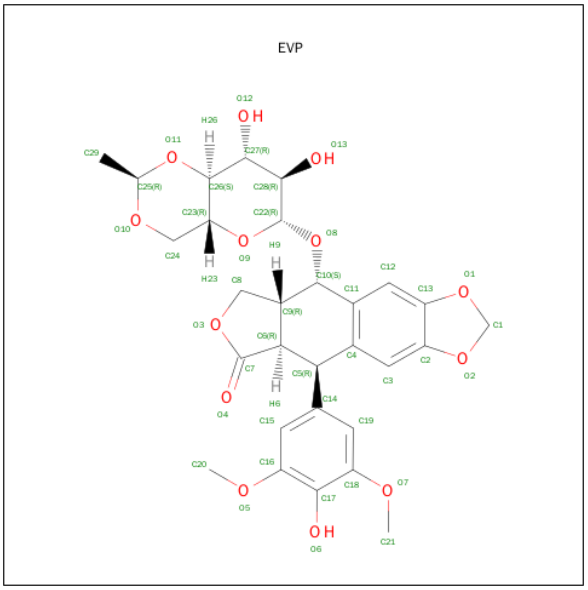


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	T	1	Total C O 6 3 3	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Na 1 1	0	0

- Molecule 9 is (5S,5aR,8aR,9R)-9-(4-hydroxy-3,5-dimethoxyphenyl)-8-oxo-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol-5-yl 4,6-O-[(1R)-ethylidene]-beta-D-glucopyranoside (three-letter code: EVP) (formula: $C_{29}H_{32}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total C O 42 29 13	0	0
9	O	1	Total C O 42 29 13	0	0
9	N	1	Total C O 42 29 13	0	0
9	P	1	Total C O 42 29 13	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	75	Total O 75 75	0	0
10	B	27	Total O 27 27	0	0
10	C	76	Total O 76 76	0	0

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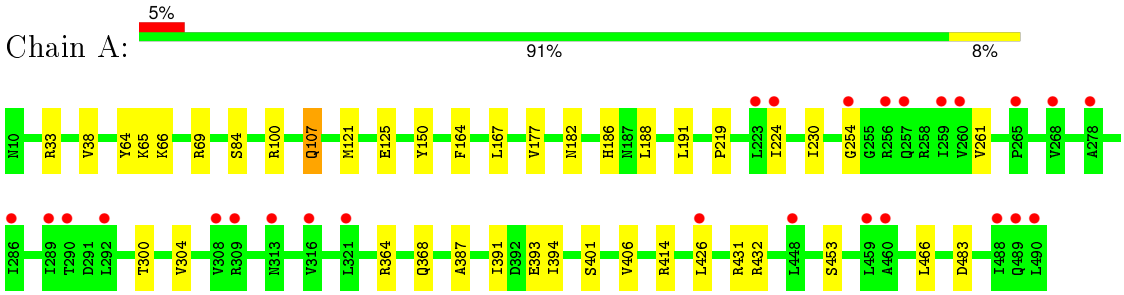
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	17	Total O 17 17	0	0
10	E	8	Total O 8 8	0	0
10	G	9	Total O 9 9	0	0
10	F	5	Total O 5 5	0	0
10	O	6	Total O 6 6	0	0
10	R	64	Total O 64 64	0	0
10	S	15	Total O 15 15	0	0
10	T	79	Total O 79 79	0	0
10	U	12	Total O 12 12	0	0
10	V	4	Total O 4 4	0	0
10	N	2	Total O 2 2	0	0
10	W	7	Total O 7 7	0	0
10	P	6	Total O 6 6	0	0

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.

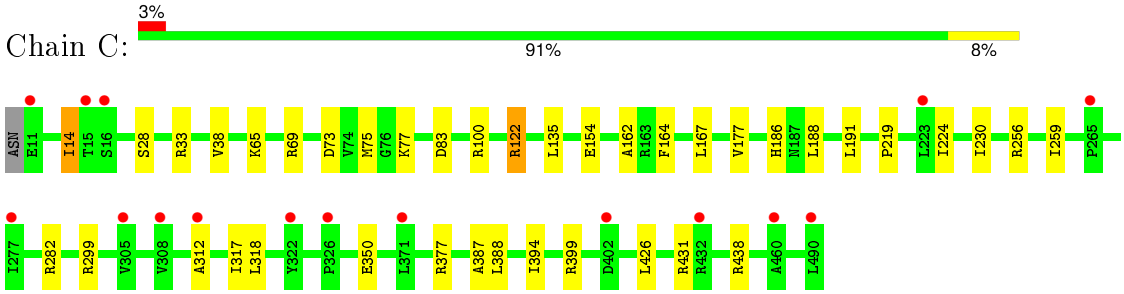
- Molecule 1: DNA gyrase subunit A

Chain A:



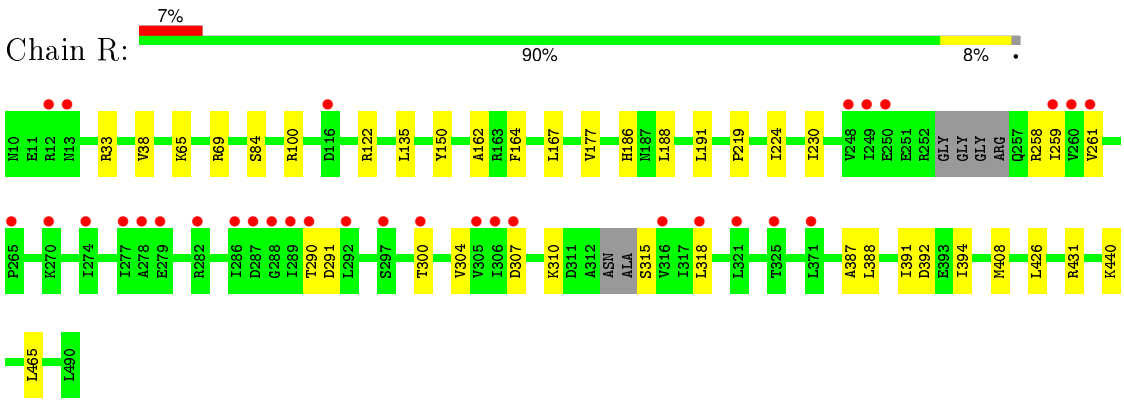
- Molecule 1: DNA gyrase subunit A

Chain C:



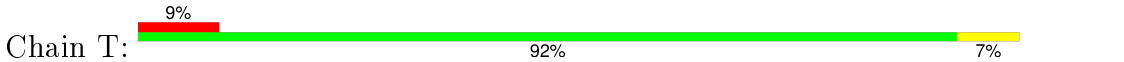
- Molecule 1: DNA gyrase subunit A

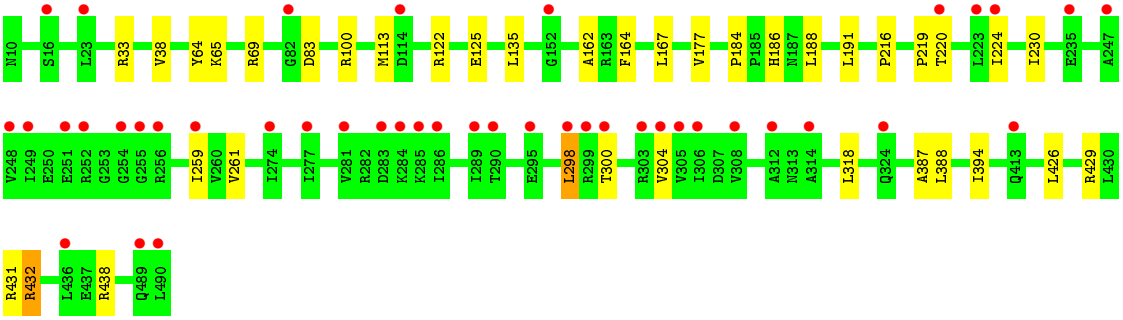
Chain R:



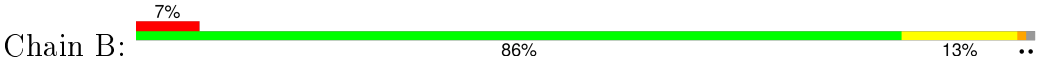
- Molecule 1: DNA gyrase subunit A

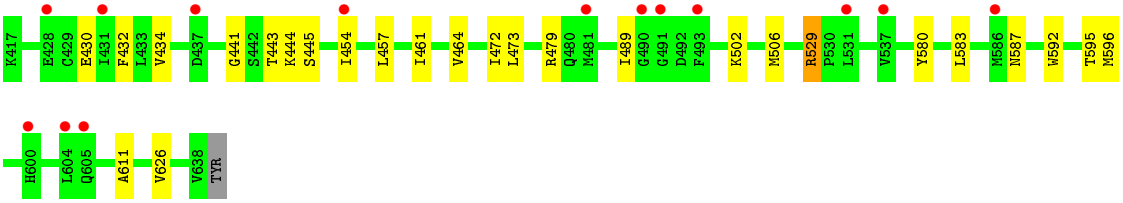
Chain T:



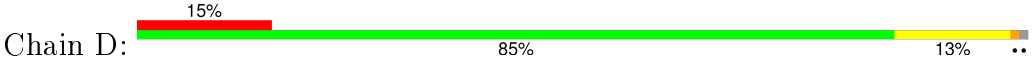


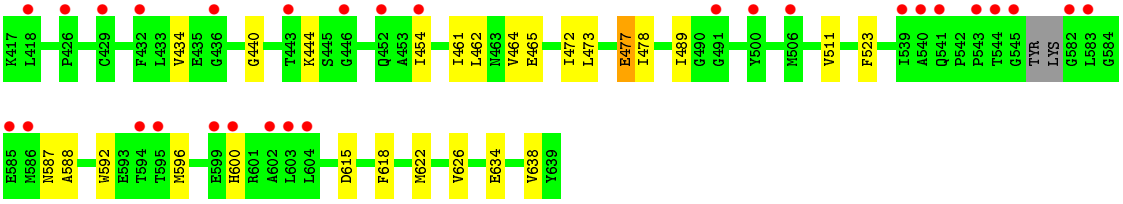
• Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



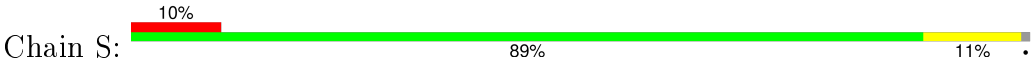


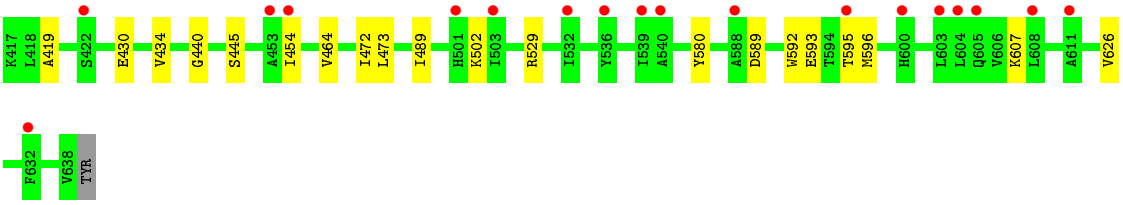
• Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



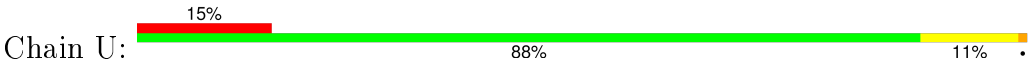


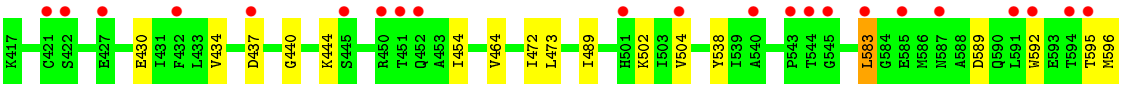
• Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B

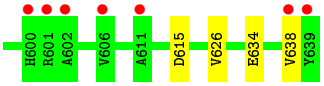




• Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B







• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP**GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3')

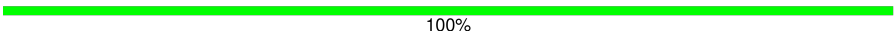
Chain E: 

There are no outlier residues recorded for this chain.

• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP**GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3')

Chain F: 

• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP**GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3')

Chain V: 

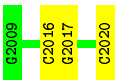
There are no outlier residues recorded for this chain.

• Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP**GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3')

Chain W: 

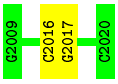
• Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3')

Chain G: 



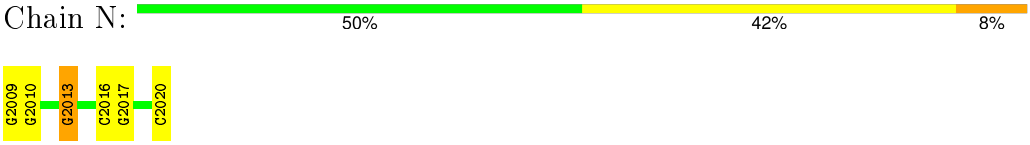
• Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*C)-3')

Chain O: 



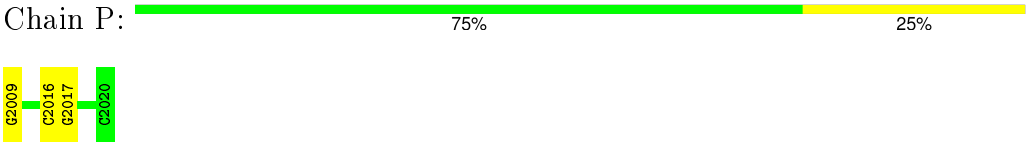
• Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*C)-3')

Chain N:



• Molecule 4: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*C*GP*GP*CP*CP*GP*TP*AP*CP *GP*CP*TP*C)-3')

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.78Å 170.08Å 124.54Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	39.35 – 2.79 39.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.1 (39.35-2.79) 96.2 (39.35-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.213 , 0.242 0.230 , 0.266	Depositor DCC
R_{free} test set	3484 reflections (4.16%)	DCC
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 87157 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23069	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NA, MN, SO4, EVP, PTR

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	0.38	0/3807	0.59	0/5135
1	C	0.38	0/3805	0.59	0/5131
1	R	0.40	0/3751	0.59	0/5062
1	T	0.39	0/3830	0.60	0/5168
2	B	0.39	0/1479	0.61	0/2000
2	D	0.39	0/1458	0.61	0/1973
2	S	0.38	0/1460	0.59	0/1975
2	U	0.39	0/1473	0.61	0/1994
3	E	0.91	0/182	0.90	0/280
3	F	0.87	0/183	0.83	0/281
3	V	0.91	0/183	0.89	0/281
3	W	0.93	0/183	0.86	0/281
4	G	1.04	0/268	0.95	0/412
4	N	1.15	1/288 (0.3%)	0.99	0/440
4	O	0.97	0/253	0.95	0/389
4	P	0.98	0/258	1.00	0/396
All	All	0.46	1/22861 (0.0%)	0.63	0/31198

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	2013	DG	O5'-C5'	-5.10	1.29	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3778	0	3768	19	0
1	C	3775	0	3799	25	0
1	R	3723	0	3720	19	0
1	T	3798	0	3777	21	0
2	B	1456	0	1413	12	0
2	D	1433	0	1376	17	0
2	S	1437	0	1388	9	0
2	U	1447	0	1400	13	0
3	E	162	0	88	0	0
3	F	163	0	91	2	0
3	V	163	0	91	0	0
3	W	163	0	91	1	0
4	G	240	0	133	4	0
4	N	259	0	145	8	0
4	O	227	0	123	2	0
4	P	231	0	126	3	0
5	A	5	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
7	C	12	0	16	1	0
7	E	6	0	8	0	0
7	T	6	0	8	0	0
8	C	1	0	0	0	0
9	G	42	0	32	0	0
9	N	42	0	32	0	0
9	O	42	0	32	0	0
9	P	42	0	32	0	0
10	A	75	0	0	1	0
10	B	27	0	0	0	0
10	C	76	0	0	1	0
10	D	17	0	0	0	0
10	E	8	0	0	0	0
10	F	5	0	0	0	0
10	G	9	0	0	0	0
10	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	O	6	0	0	0	0
10	P	6	0	0	0	0
10	R	64	0	0	0	0
10	S	15	0	0	0	0
10	T	79	0	0	0	0
10	U	12	0	0	0	0
10	V	4	0	0	0	0
10	W	7	0	0	0	0
All	All	23069	0	21689	127	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 (127) 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:R:388:LEU:HD23	1:R:391:ILE:HD11	1.70	0.73
1:A:401:SER:HB3	1:A:406:VAL:HG23	1.73	0.71
4:G:2020:DC:H2"	3:F:1:DG:H1	1.57	0.70
2:U:502:LYS:HG2	2:U:538:TYR:HE2	1.56	0.70
2:B:432:PHE:HB2	2:B:454:ILE:CD1	2.23	0.69
4:N:2013:DG:H5"	4:N:2013:DG:C8	2.36	0.61
1:C:122:ARG:H	1:C:122:ARG:HD3	1.65	0.60
2:S:589:ASP:CB	1:T:298:LEU:HD12	2.31	0.60
4:N:2013:DG:H8	4:N:2013:DG:H5"	1.66	0.59
1:A:66:LYS:HB3	10:A:601:HOH:O	2.01	0.59
2:B:432:PHE:HB2	2:B:454:ILE:HD13	1.84	0.59
1:R:426:LEU:HB3	1:T:431:ARG:HB3	1.84	0.59
4:G:2020:DC:H2"	3:F:1:DG:N1	2.18	0.58
2:D:461:ILE:HD13	2:D:477:GLU:HB3	1.85	0.58
1:C:14:ILE:CD1	2:D:618:PHE:HZ	2.15	0.58
2:B:457:LEU:HB3	2:B:461:ILE:HD11	1.86	0.58
1:R:291:ASP:H	1:R:307:ASP:HB2	1.68	0.57
2:U:437:ASP:HB2	4:N:2010:DG:OP1	2.05	0.57
1:R:388:LEU:HA	1:R:391:ILE:HD11	1.86	0.57
1:C:73:ASP:O	1:C:77:LYS:HG2	2.06	0.56
1:T:64:TYR:HB3	1:T:125:GLU:HB3	1.88	0.56
1:C:224:ILE:HG21	1:C:230:ILE:HD11	1.88	0.56
1:T:224:ILE:HG21	1:T:230:ILE:HD11	1.87	0.55
1:R:224:ILE:HG21	1:R:230:ILE:HD11	1.89	0.53
1:A:224:ILE:HG21	1:A:230:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:626:VAL:HG11	4:P:2017:DG:H3'	1.92	0.52
1:T:113:MET:CE	1:T:220:THR:HG22	2.40	0.52
1:C:388:LEU:HD22	1:C:438:ARG:HG2	1.92	0.51
1:C:387:ALA:HA	1:C:394:ILE:HG13	1.92	0.51
1:A:426:LEU:HB3	1:C:431:ARG:HB3	1.92	0.51
2:S:473:LEU:HD21	2:S:489:ILE:HD11	1.92	0.51
2:D:434:VAL:HG21	2:D:440:GLY:HA2	1.93	0.50
2:D:626:VAL:HG11	4:O:2017:DG:H3'	1.94	0.49
2:U:502:LYS:HG2	2:U:538:TYR:CE2	2.44	0.49
1:R:431:ARG:HB3	1:T:426:LEU:HB3	1.94	0.49
1:C:377:ARG:HH22	7:C:503:GOL:H12	1.77	0.49
2:B:473:LEU:HD21	2:B:489:ILE:HD11	1.95	0.49
4:N:2020[B]:DC:H2'	3:W:1:DG:O6	2.11	0.49
1:R:177:VAL:HG22	4:N:2016:DC:H4'	1.92	0.49
1:C:312:ALA:HB1	1:C:317:ILE:HD11	1.95	0.49
2:D:592:TRP:HA	2:D:596:MET:HB2	1.95	0.49
2:U:434:VAL:HG21	2:U:440:GLY:HA2	1.93	0.49
2:S:626:VAL:HG11	4:N:2017:DG:H3'	1.94	0.49
1:C:77:LYS:HB2	1:C:154:GLU:HG3	1.95	0.48
1:A:393:GLU:HB3	1:A:414:ARG:HH11	1.78	0.48
1:A:150:TYR:HD2	2:B:580:TYR:HB2	1.78	0.48
1:T:122[B]:ARG:H	1:T:122[B]:ARG:HD3	1.79	0.48
1:A:64:TYR:HB3	1:A:125:GLU:HB3	1.95	0.48
1:A:391:ILE:HG21	1:C:399:ARG:HD3	1.95	0.47
1:T:388:LEU:HD22	1:T:438:ARG:HG2	1.95	0.47
1:R:100:ARG:HA	1:R:219:PRO:HB3	1.97	0.47
1:T:387:ALA:HA	1:T:394:ILE:HG13	1.94	0.47
1:R:150:TYR:HD2	2:S:580:TYR:HB2	1.78	0.47
2:S:592:TRP:HA	2:S:596:MET:HB2	1.96	0.47
2:S:434:VAL:HG21	2:S:440:GLY:HA2	1.95	0.47
1:A:364:ARG:HG2	1:A:368:GLN:HE21	1.79	0.47
1:R:388:LEU:HA	1:R:391:ILE:CD1	2.45	0.47
1:T:177:VAL:HG22	4:P:2016:DC:H4'	1.97	0.47
2:U:473:LEU:HD21	2:U:489:ILE:HD11	1.97	0.47
1:A:387:ALA:HA	1:A:394:ILE:HG13	1.96	0.47
1:C:100:ARG:HA	1:C:219:PRO:HB3	1.97	0.47
1:A:431:ARG:HB3	1:C:426:LEU:HB3	1.96	0.47
1:R:122:ARG:NH2	4:N:2009:DG:H2'	2.31	0.46
1:T:122[B]:ARG:HH22	4:P:2009:DG:H2'	1.79	0.46
2:U:592:TRP:HA	2:U:596:MET:HB2	1.97	0.46
1:R:387:ALA:HA	1:R:394:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:504:VAL:HG22	2:U:538:TYR:HB2	1.98	0.46
1:C:14:ILE:CD1	2:D:618:PHE:CZ	2.98	0.46
2:B:592:TRP:HA	2:B:596:MET:HB2	1.97	0.46
2:D:473:LEU:HD21	2:D:489:ILE:HD11	1.97	0.45
1:A:177:VAL:HG22	4:G:2016:DC:H4'	1.98	0.45
1:R:164:PHE:HB2	1:R:188:LEU:HD11	1.98	0.45
2:D:461:ILE:HD11	2:D:478:ILE:HG12	1.99	0.45
2:B:506:MET:HG2	2:B:583:LEU:HD21	1.98	0.45
2:U:634:GLU:HA	2:U:638:VAL:HB	1.98	0.45
1:A:65:LYS:HE2	1:A:69:ARG:HB3	1.99	0.45
1:A:100:ARG:HA	1:A:219:PRO:HB3	1.98	0.45
1:C:186:HIS:HB2	1:C:191:LEU:HD11	1.98	0.44
1:A:186:HIS:HB2	1:A:191:LEU:HD11	2.00	0.44
1:T:186:HIS:HB2	1:T:191:LEU:HD11	1.99	0.44
2:D:464:VAL:HG12	2:D:472:ILE:HG12	2.00	0.44
1:C:14:ILE:HD12	2:D:618:PHE:HZ	1.83	0.44
1:C:177:VAL:HG22	4:O:2016:DC:H4'	2.00	0.44
1:C:164:PHE:HB2	1:C:188:LEU:HD11	1.99	0.44
2:B:430:GLU:HB3	2:B:502:LYS:HB2	2.00	0.44
1:T:65:LYS:HE2	1:T:69:ARG:HB3	2.00	0.44
1:R:65:LYS:HE2	1:R:69:ARG:HB3	2.00	0.43
2:U:444:LYS:HA	2:U:454:ILE:HD13	2.00	0.43
2:U:430:GLU:HB3	2:U:502:LYS:HB2	2.00	0.43
2:D:634:GLU:HA	2:D:638:VAL:HB	2.00	0.43
1:C:350:GLU:HG2	10:C:608:HOH:O	2.18	0.43
2:D:465:GLU:HG3	2:D:622:MET:HB2	2.00	0.43
2:S:430:GLU:HB3	2:S:502:LYS:HB2	2.00	0.43
1:A:164:PHE:HB2	1:A:188:LEU:HD11	1.99	0.43
2:D:461:ILE:HD12	2:D:462:LEU:H	1.84	0.43
2:U:464:VAL:HG12	2:U:472:ILE:HG12	2.00	0.43
2:D:444:LYS:HA	2:D:454:ILE:HD13	2.01	0.43
1:R:186:HIS:HB2	1:R:191:LEU:HD11	1.99	0.43
1:T:429:ARG:H	1:T:432:ARG:HH21	1.66	0.43
1:C:65:LYS:HE2	1:C:69:ARG:HB3	1.99	0.43
2:B:626:VAL:HG11	4:G:2017:DG:H3'	2.01	0.43
1:T:38:VAL:HA	1:T:167:LEU:HD22	2.01	0.43
2:S:419:ALA:HB3	2:S:454:ILE:HG13	2.01	0.42
1:C:38:VAL:HA	1:C:167:LEU:HD22	2.01	0.42
1:R:135:LEU:HA	1:R:162:ALA:HA	2.01	0.42
1:A:38:VAL:HA	1:A:167:LEU:HD22	2.01	0.42
1:T:100:ARG:HA	1:T:219:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:464:VAL:HG12	2:S:472:ILE:HG12	2.01	0.42
2:B:464:VAL:HG12	2:B:472:ILE:HG12	2.01	0.42
1:T:164:PHE:HB2	1:T:188:LEU:HD11	2.00	0.42
2:B:529:ARG:HH21	2:B:611:ALA:HB1	1.84	0.42
2:D:464:VAL:HG21	2:D:523:PHE:HA	2.02	0.41
1:A:107:GLN:HB3	1:A:125:GLU:HB2	2.03	0.41
1:C:259:ILE:HG21	1:C:318:LEU:HD13	2.01	0.41
1:R:259:ILE:HG21	1:R:318:LEU:HD13	2.03	0.41
1:C:14:ILE:HD12	2:D:618:PHE:CZ	2.56	0.41
1:R:38:VAL:HA	1:R:167:LEU:HD22	2.02	0.41
1:T:259:ILE:HG21	1:T:318:LEU:HD13	2.01	0.41
2:U:437:ASP:CB	4:N:2010:DG:OP1	2.68	0.41
1:R:261:VAL:HB	1:R:304:VAL:HB	2.03	0.41
2:B:441:GLY:HA2	2:B:444:LYS:HG2	2.03	0.41
1:T:184:PRO:HB2	1:T:216:PRO:HB3	2.03	0.40
1:C:28:SER:HB2	2:D:511:VAL:HG11	2.03	0.40
1:A:261:VAL:HB	1:A:304:VAL:HB	2.03	0.40
1:T:135:LEU:HA	1:T:162:ALA:HA	2.04	0.40
1:T:261:VAL:HB	1:T:304:VAL:HB	2.03	0.40
1:C:135:LEU:HA	1:C:162:ALA:HA	2.04	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	480/481 (100%)	463 (96%)	14 (3%)	3 (1%)	30 65
1	C	477/481 (99%)	462 (97%)	14 (3%)	1 (0%)	52 84
1	R	468/481 (97%)	451 (96%)	15 (3%)	2 (0%)	39 74
1	T	483/481 (100%)	464 (96%)	18 (4%)	1 (0%)	52 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	186/189 (98%)	183 (98%)	3 (2%)	0	100 100
2	D	184/189 (97%)	177 (96%)	6 (3%)	1 (0%)	34 69
2	S	186/189 (98%)	183 (98%)	3 (2%)	0	100 100
2	U	188/189 (100%)	180 (96%)	7 (4%)	1 (0%)	34 69
All	All	2652/2680 (99%)	2563 (97%)	80 (3%)	9 (0%)	46 79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	310	LYS
2	U	583	LEU
2	D	588	ALA
1	A	33	ARG
1	C	33	ARG
1	R	33	ARG
1	T	33	ARG
1	A	121	MET
1	A	254	GLY

5.3.2 Protein sidechains (i)

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	401/415 (97%)	393 (98%)	8 (2%)	63 90
1	C	404/415 (97%)	397 (98%)	7 (2%)	68 92
1	R	396/415 (95%)	387 (98%)	9 (2%)	58 88
1	T	403/415 (97%)	399 (99%)	4 (1%)	82 96
2	B	152/158 (96%)	145 (95%)	7 (5%)	33 67
2	D	146/158 (92%)	142 (97%)	4 (3%)	52 85
2	S	146/158 (92%)	141 (97%)	5 (3%)	44 78
2	U	147/158 (93%)	143 (97%)	4 (3%)	52 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2195/2292 (96%)	2147 (98%)	48 (2%)	60 89

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	107	GLN
1	A	182	ASN
1	A	300	THR
1	A	432	ARG
1	A	453	SER
1	A	466	LEU
1	A	483	ASP
2	B	434	VAL
2	B	443	THR
2	B	445	SER
2	B	479	ARG
2	B	529	ARG
2	B	587	ASN
2	B	595	THR
1	C	14	ILE
1	C	75	MET
1	C	83	ASP
1	C	122	ARG
1	C	256	ARG
1	C	282	ARG
1	C	299	ARG
2	D	477	GLU
2	D	587	ASN
2	D	600	HIS
2	D	615	ASP
1	R	84	SER
1	R	258	ARG
1	R	290	THR
1	R	300	THR
1	R	315	SER
1	R	392	ASP
1	R	408	MET
1	R	440	LYS
1	R	465	LEU
2	S	445	SER
2	S	529	ARG

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Mol	Chain	Res	Type
2	S	593	GLU
2	S	595	THR
2	S	607	LYS
1	T	83	ASP
1	T	298	LEU
1	T	300	THR
1	T	432	ARG
2	U	583	LEU
2	U	589	ASP
2	U	595	THR
2	U	615	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	368	GLN
2	D	476	ASN
2	D	480	GLN
2	D	597	ASN
2	D	600	HIS
2	S	628	ASN
1	T	54	ASN
1	T	153	ASN

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	PTR	A	123	1	13,16,17	1.78	4 (30%)	19,22,24	2.02	7 (36%)
1	PTR	C	123	1	13,16,17	1.44	1 (7%)	19,22,24	1.49	4 (21%)
1	PTR	R	123	1,4	13,16,17	1.34	1 (7%)	19,22,24	1.18	1 (5%)
1	PTR	T	123	1,4	13,16,17	1.14	1 (7%)	19,22,24	1.40	3 (15%)

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	PTR	A	123	1	-	0/9/11/13	0/1/1/1
1	PTR	C	123	1	-	0/9/11/13	0/1/1/1
1	PTR	R	123	1,4	-	0/9/11/13	0/1/1/1
1	PTR	T	123	1,4	-	0/9/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	123	PTR	CE1-CZ	2.07	1.42	1.38
1	A	123	PTR	CE1-CZ	2.19	1.43	1.38
1	A	123	PTR	CD2-CG	2.61	1.44	1.38
1	R	123	PTR	CE1-CZ	2.73	1.44	1.38
1	A	123	PTR	CE2-CD2	3.13	1.45	1.38
1	C	123	PTR	CE1-CZ	3.15	1.45	1.38
1	A	123	PTR	CE2-CZ	3.78	1.46	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	PTR	O3P-P-O1P	-4.89	94.67	110.63
1	A	123	PTR	P-OH-CZ	-2.97	115.42	123.85
1	C	123	PTR	O-C-CA	-2.54	118.90	125.72
1	A	123	PTR	CB-CG-CD1	-2.49	115.89	120.91
1	C	123	PTR	O3P-P-O1P	-2.43	102.71	110.63
1	T	123	PTR	O-C-CA	-2.41	119.25	125.72
1	A	123	PTR	O-C-CA	-2.33	119.46	125.72
1	R	123	PTR	O-C-CA	-2.32	119.50	125.72
1	T	123	PTR	CD2-CG-CD1	2.08	121.58	118.15
1	C	123	PTR	O2P-P-OH	2.09	112.12	105.47
1	A	123	PTR	O2P-P-OH	2.32	112.87	105.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	PTR	O3P-P-OH	2.44	113.26	105.47
1	A	123	PTR	CD1-CE1-CZ	2.56	122.94	119.74
1	C	123	PTR	O3P-P-OH	2.75	114.23	105.47
1	T	123	PTR	O2P-P-OH	3.72	117.33	105.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.12	0
7	GOL	C	501	-	5,5,5	0.11	0	5,5,5	0.18	0
7	GOL	C	503	-	5,5,5	0.10	0	5,5,5	0.30	0
7	GOL	E	101	-	5,5,5	0.10	0	5,5,5	0.40	0
9	EVP	G	2101	-	48,48,48	0.77	1 (2%)	70,73,73	2.01	19 (27%)
9	EVP	N	2101	-	48,48,48	0.76	1 (2%)	70,73,73	1.93	13 (18%)
9	EVP	O	2101	-	48,48,48	0.78	1 (2%)	70,73,73	1.79	16 (22%)
9	EVP	P	2101	-	48,48,48	0.81	1 (2%)	70,73,73	2.14	15 (21%)
7	GOL	T	501	-	5,5,5	0.12	0	5,5,5	0.18	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
5	SO4	A	501	-	-	0/0/0/0	0/0/0/0
7	GOL	C	501	-	-	0/4/4/4	0/0/0/0
7	GOL	C	503	-	-	0/4/4/4	0/0/0/0
7	GOL	E	101	-	-	0/4/4/4	0/0/0/0
9	EVP	G	2101	-	-	0/12/76/76	0/7/7/7
9	EVP	N	2101	-	-	0/12/76/76	0/7/7/7
9	EVP	O	2101	-	-	0/12/76/76	0/7/7/7
9	EVP	P	2101	-	-	0/12/76/76	0/7/7/7
7	GOL	T	501	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	2101	EVP	C6-C9	-2.32	1.49	1.54
9	P	2101	EVP	C6-C9	-2.27	1.50	1.54
9	G	2101	EVP	C6-C9	-2.16	1.50	1.54
9	N	2101	EVP	C6-C9	-2.00	1.50	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	2101	EVP	C20-O5-C16	-7.21	107.00	117.53
9	G	2101	EVP	C20-O5-C16	-7.16	107.08	117.53
9	N	2101	EVP	C20-O5-C16	-6.69	107.77	117.53
9	P	2101	EVP	C11-C10-C9	-5.15	106.28	111.53
9	O	2101	EVP	C20-O5-C16	-5.11	110.07	117.53
9	P	2101	EVP	C1-O2-C2	-4.99	98.04	105.32
9	G	2101	EVP	C21-O7-C18	-4.93	110.34	117.53
9	O	2101	EVP	C11-C10-C9	-4.85	106.59	111.53
9	P	2101	EVP	C21-O7-C18	-4.84	110.46	117.53
9	P	2101	EVP	C1-O1-C13	-4.76	98.37	105.32
9	O	2101	EVP	C21-O7-C18	-4.51	110.95	117.53
9	N	2101	EVP	C21-O7-C18	-4.49	110.97	117.53
9	N	2101	EVP	C11-C10-C9	-4.40	107.05	111.53
9	N	2101	EVP	C1-O2-C2	-4.37	98.94	105.32
9	G	2101	EVP	C1-O2-C2	-4.06	99.40	105.32
9	G	2101	EVP	C1-O1-C13	-4.04	99.42	105.32
9	N	2101	EVP	C1-O1-C13	-4.00	99.48	105.32
9	G	2101	EVP	C11-C10-C9	-3.90	107.55	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	2101	EVP	C1-O2-C2	-3.85	99.70	105.32
9	O	2101	EVP	C1-O1-C13	-3.77	99.82	105.32
9	P	2101	EVP	O5-C16-C15	-3.01	118.99	124.17
9	O	2101	EVP	C22-O9-C23	-2.72	108.41	113.74
9	G	2101	EVP	O5-C16-C15	-2.69	119.55	124.17
9	N	2101	EVP	O5-C16-C15	-2.65	119.61	124.17
9	P	2101	EVP	O4-C7-C6	-2.64	126.31	129.49
9	O	2101	EVP	C24-O10-C25	-2.58	109.19	111.62
9	G	2101	EVP	O4-C7-C6	-2.54	126.43	129.49
9	O	2101	EVP	O4-C7-C6	-2.45	126.54	129.49
9	P	2101	EVP	C22-O9-C23	-2.44	108.95	113.74
9	G	2101	EVP	C22-O8-C10	-2.42	110.80	115.53
9	P	2101	EVP	C24-O10-C25	-2.35	109.41	111.62
9	G	2101	EVP	C24-O10-C25	-2.18	109.56	111.62
9	N	2101	EVP	O4-C7-C6	-2.03	127.04	129.49
9	G	2101	EVP	C8-C9-C6	2.01	104.25	101.65
9	G	2101	EVP	C4-C5-C6	2.03	110.10	106.58
9	G	2101	EVP	O1-C13-C2	2.10	112.38	109.77
9	O	2101	EVP	O1-C13-C2	2.12	112.40	109.77
9	G	2101	EVP	O2-C2-C13	2.12	112.41	109.77
9	G	2101	EVP	C22-C28-C27	2.13	114.21	109.98
9	P	2101	EVP	O2-C2-C13	2.26	112.58	109.77
9	O	2101	EVP	O11-C25-O10	2.29	112.94	110.80
9	O	2101	EVP	O2-C2-C13	2.32	112.66	109.77
9	N	2101	EVP	O2-C2-C13	2.37	112.72	109.77
9	G	2101	EVP	O3-C7-O4	2.39	124.11	121.44
9	O	2101	EVP	O3-C7-O4	2.58	124.33	121.44
9	N	2101	EVP	O3-C7-O4	2.72	124.48	121.44
9	P	2101	EVP	O2-C1-O1	2.86	113.00	108.09
9	N	2101	EVP	O7-C18-C17	3.06	117.57	114.47
9	O	2101	EVP	O5-C16-C17	3.06	117.58	114.47
9	P	2101	EVP	O3-C7-O4	3.12	124.93	121.44
9	N	2101	EVP	O2-C1-O1	3.13	113.45	108.09
9	G	2101	EVP	O2-C1-O1	3.20	113.58	108.09
9	P	2101	EVP	C11-C4-C5	3.28	122.83	114.26
9	G	2101	EVP	C11-C4-C5	3.29	122.85	114.26
9	N	2101	EVP	C11-C4-C5	3.31	122.92	114.26
9	O	2101	EVP	C11-C4-C5	3.35	123.02	114.26
9	O	2101	EVP	O7-C18-C17	3.46	117.98	114.47
9	O	2101	EVP	O2-C1-O1	3.64	114.32	108.09
9	G	2101	EVP	O7-C18-C17	3.75	118.28	114.47
9	P	2101	EVP	O7-C18-C17	4.55	119.09	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	2101	EVP	O5-C16-C17	5.91	120.47	114.47
9	N	2101	EVP	O5-C16-C17	5.92	120.49	114.47
9	P	2101	EVP	O5-C16-C17	6.30	120.87	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	503	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	480/481 (99%)	0.47	26 (5%) 29 19	48, 69, 101, 115	0
1	C	479/481 (99%)	0.43	16 (3%) 50 38	43, 65, 95, 132	0
1	R	474/481 (98%)	0.53	32 (6%) 20 12	45, 70, 120, 155	0
1	T	480/481 (99%)	0.54	43 (8%) 12 6	47, 70, 125, 152	0
2	B	188/189 (99%)	0.68	14 (7%) 17 9	53, 85, 112, 121	0
2	D	187/189 (98%)	1.09	29 (15%) 3 1	49, 95, 142, 161	0
2	S	188/189 (99%)	0.80	18 (9%) 10 5	62, 102, 134, 149	0
2	U	189/189 (100%)	0.85	29 (15%) 3 1	58, 90, 125, 144	0
3	E	8/8 (100%)	0.47	0 100 100	52, 64, 76, 78	0
3	F	8/8 (100%)	0.44	0 100 100	52, 59, 87, 93	0
3	V	8/8 (100%)	0.48	0 100 100	54, 63, 86, 88	0
3	W	8/8 (100%)	0.34	0 100 100	56, 66, 91, 99	0
4	G	12/12 (100%)	0.09	0 100 100	54, 74, 89, 91	0
4	N	12/12 (100%)	0.09	0 100 100	61, 76, 93, 98	0
4	O	12/12 (100%)	0.31	0 100 100	53, 66, 90, 93	0
4	P	12/12 (100%)	-0.09	0 100 100	56, 76, 88, 93	0
All	All	2745/2760 (99%)	0.58	207 (7%) 17 9	43, 73, 121, 161	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	587	ASN	6.8
2	D	585	GLU	6.3
1	R	259	ILE	6.1
2	D	586	MET	5.3
1	T	305	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	539	ILE	5.1
2	D	545	GLY	5.1
2	U	437	ASP	5.0
2	D	604	LEU	5.0
2	D	544	THR	5.0
1	R	260	VAL	4.9
2	U	639	TYR	4.8
2	D	602	ALA	4.7
1	R	289	ILE	4.7
2	U	600	HIS	4.7
2	U	592	TRP	4.6
2	D	583	LEU	4.6
1	T	223	LEU	4.5
1	R	261	VAL	4.5
2	D	599	GLU	4.5
1	T	254	GLY	4.5
2	D	600	HIS	4.4
1	T	300	THR	4.3
2	B	491	GLY	4.3
1	T	247	ALA	4.3
1	A	259	ILE	4.2
1	R	277	ILE	4.1
2	U	583	LEU	4.1
1	T	255	GLY	4.1
2	S	501	HIS	4.1
2	U	544	THR	4.0
1	T	289	ILE	3.8
1	A	308	VAL	3.8
2	U	545	GLY	3.8
1	A	223	LEU	3.7
2	S	588	ALA	3.7
1	C	490	LEU	3.7
1	T	308	VAL	3.7
2	B	490	GLY	3.7
2	D	491	GLY	3.7
1	T	285	LYS	3.7
1	R	278	ALA	3.6
2	S	605	GLN	3.6
1	R	250	GLU	3.6
2	S	608	LEU	3.6
1	A	260	VAL	3.6
2	B	604	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	292	LEU	3.5
2	D	454	ILE	3.5
2	D	540	ALA	3.5
1	T	281	VAL	3.5
1	T	16	SER	3.4
1	R	286	ILE	3.4
1	A	289	ILE	3.4
2	S	539	ILE	3.3
2	D	543	PRO	3.3
1	C	326	PRO	3.3
2	U	611	ALA	3.3
1	A	313	ASN	3.3
2	S	600	HIS	3.3
1	T	284	LYS	3.3
1	C	460	ALA	3.2
2	S	604	LEU	3.2
2	S	503	ILE	3.2
1	C	223	LEU	3.2
1	R	305	VAL	3.2
1	T	256	ARG	3.2
1	T	283	ASP	3.2
1	R	321	LEU	3.2
1	R	307	ASP	3.1
2	D	443	THR	3.1
1	C	308	VAL	3.1
1	R	292	LEU	3.1
1	R	297	SER	3.1
1	R	282	ARG	3.1
1	T	413	GLN	3.1
2	B	454	ILE	3.0
2	D	594	THR	3.0
1	C	305	VAL	3.0
1	R	116	ASP	3.0
2	U	638	VAL	3.0
1	T	299	ARG	3.0
2	U	601	ARG	3.0
2	D	429	CYS	3.0
1	C	312	ALA	3.0
1	C	277	ILE	3.0
1	R	316	VAL	3.0
2	U	585	GLU	3.0
1	C	402	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	493	PHE	2.9
1	R	300	THR	2.9
1	R	306	ILE	2.9
1	T	306	ILE	2.9
2	B	431	ILE	2.9
2	D	432	PHE	2.9
1	R	270	LYS	2.9
1	R	290	THR	2.9
2	U	450	ARG	2.9
1	T	277	ILE	2.9
1	T	298	LEU	2.9
1	R	325	THR	2.9
1	T	286	ILE	2.8
2	D	541	GLN	2.8
1	A	224	ILE	2.8
2	B	428	GLU	2.8
2	S	603	LEU	2.8
2	B	437	ASP	2.8
2	S	611	ALA	2.7
2	B	586	MET	2.7
1	T	259	ILE	2.7
2	D	603	LEU	2.7
2	U	591	LEU	2.7
2	S	595	THR	2.7
2	U	422	SER	2.7
2	D	446	GLY	2.7
1	T	251	GLU	2.7
1	T	274	ILE	2.7
1	C	16	SER	2.7
1	A	278	ALA	2.7
1	T	314	ALA	2.7
1	R	248	VAL	2.6
1	A	321	LEU	2.6
1	C	15	THR	2.6
1	T	248	VAL	2.6
2	D	500	TYR	2.5
1	A	265	PRO	2.5
1	T	220	THR	2.5
2	U	543	PRO	2.5
1	A	268	VAL	2.5
2	S	632	PHE	2.5
1	T	303	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	T	489	GLN	2.5
1	A	309	ARG	2.5
1	T	324	GLN	2.4
2	U	594	THR	2.4
1	A	316	VAL	2.4
2	U	504	VAL	2.4
2	D	426	PRO	2.4
1	T	249	ILE	2.4
2	B	481	MET	2.4
1	T	290	THR	2.4
2	S	422	SER	2.4
2	U	595	THR	2.4
2	U	432	PHE	2.4
1	T	295	GLU	2.4
2	B	605	GLN	2.4
2	D	418	LEU	2.4
2	D	595	THR	2.4
1	T	224	ILE	2.4
2	S	532	ILE	2.4
1	R	279	GLU	2.4
1	C	371	LEU	2.3
1	T	235	GLU	2.3
2	U	501	HIS	2.3
2	S	536	TYR	2.3
2	U	451	THR	2.3
2	U	540	ALA	2.3
1	R	288	GLY	2.3
1	T	252	ARG	2.3
2	U	445	SER	2.3
1	A	460	ALA	2.3
1	T	304	VAL	2.3
1	C	11	GLU	2.3
1	A	448	LEU	2.3
2	S	540	ALA	2.3
1	A	488	ILE	2.3
1	T	312	ALA	2.2
2	U	602	ALA	2.2
1	R	274	ILE	2.2
1	T	152	GLY	2.2
1	A	490	LEU	2.2
1	T	490	LEU	2.2
1	A	290	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	322	TYR	2.2
1	A	254	GLY	2.2
1	R	249	ILE	2.2
2	S	453	ALA	2.2
2	B	537	VAL	2.2
2	S	454	ILE	2.2
2	U	452	GLN	2.2
2	U	606	VAL	2.2
1	A	489	GLN	2.2
1	T	23	LEU	2.2
2	U	421	CYS	2.2
1	R	13	ASN	2.1
2	U	427	GLU	2.1
1	T	82	GLY	2.1
2	D	436	GLY	2.1
1	A	286	ILE	2.1
1	A	426	LEU	2.1
1	A	459	LEU	2.1
1	C	432	ARG	2.1
1	R	318	LEU	2.1
1	C	265	PRO	2.1
1	R	371	LEU	2.1
1	R	287	ASP	2.1
1	A	257	GLN	2.1
2	D	582	GLY	2.1
2	B	600	HIS	2.0
1	R	265	PRO	2.0
1	T	114	ASP	2.0
2	D	452	GLN	2.0
1	T	436	LEU	2.0
1	A	256	ARG	2.0
1	R	12	ARG	2.0
2	D	506	MET	2.0
2	B	531	LEU	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^{th} 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
1	PTR	T	123	16/17	0.96	0.21	-	63,67,77,79	0
1	PTR	A	123	16/17	0.89	0.22	-	71,82,98,99	0
1	PTR	C	123	16/17	0.94	0.18	-	65,73,84,85	0
1	PTR	R	123	16/17	0.89	0.20	-	70,80,94,94	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^{th} 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
7	GOL	E	101	6/6	0.90	0.44	6.25	80,82,83,84	0
7	GOL	C	501	6/6	0.81	0.37	4.48	76,81,82,83	0
5	SO4	A	501	5/5	0.87	0.25	2.27	113,114,115,115	0
7	GOL	C	503	6/6	0.75	0.34	1.47	66,72,74,75	0
7	GOL	T	501	6/6	0.89	0.23	1.02	57,58,59,61	0
9	EVP	P	2101	42/42	0.89	0.23	-0.20	73,82,92,94	0
9	EVP	O	2101	42/42	0.90	0.21	-0.38	81,86,91,96	0
9	EVP	N	2101	42/42	0.95	0.17	-0.91	63,69,75,76	0
9	EVP	G	2101	42/42	0.94	0.17	-0.99	62,73,83,86	0
8	NA	C	502	1/1	0.86	0.19	-1.11	61,61,61,61	0
6	MN	D	1001	1/1	0.99	0.15	-	84,84,84,84	0
6	MN	U	1001	1/1	0.99	0.16	-	64,64,64,64	0
6	MN	B	1001	1/1	0.98	0.17	-	57,57,57,57	0
6	MN	S	6001	1/1	1.00	0.19	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.