



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:42 am BST

PDB ID : 6FQV
Title : 2.60A BINARY COMPLEX OF S.AUREUS GYRASE with UNCLEAVED DNA
Authors : Bax, B.D.; Germe, T.; Basque, E.; Maxwell, A.
Deposited on : 2018-02-14
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

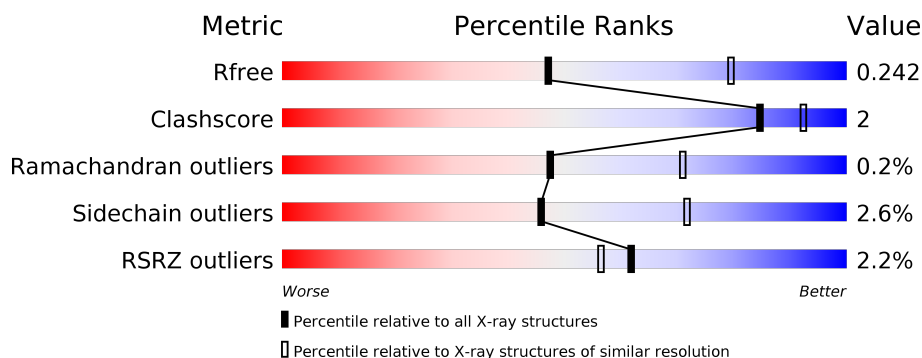
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> <div></div> </div>
1	C	490	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> <div></div> </div>
1	R	490	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> <div></div> </div>
1	T	490	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> <div></div> </div>
2	B	202	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> <div></div> </div>
2	D	202	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
2	S	202	<div><div></div><div>3%</div><div>85%</div><div>8%</div><div>6%</div></div>
2	U	202	<div><div></div><div>%</div><div>86%</div><div>9%</div><div>5%</div></div>
3	E	20	<div><div></div><div>5%</div><div>85%</div><div>15%</div></div>
3	F	20	<div><div></div><div>15%</div><div>90%</div><div>10%</div></div>
3	V	20	<div><div></div><div>85%</div><div>15%</div></div>
3	W	20	<div><div></div><div>75%</div><div>20%</div><div>5%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23182 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	482	Total	C	N	O	S	0	6	0
			3833	2389	695	731	18			
1	C	473	Total	C	N	O	S	0	2	0
			3718	2316	674	712	16			
1	R	482	Total	C	N	O	S	0	5	0
			3803	2362	692	732	17			
1	T	482	Total	C	N	O	S	0	4	0
			3819	2375	704	724	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	1	0
			1456	912	252	283	9			
2	D	189	Total	C	N	O	S	0	0	0
			1426	898	241	278	9			
2	S	189	Total	C	N	O	S	0	4	0
			1498	943	260	286	9			
2	U	192	Total	C	N	O	S	0	2	0
			1514	951	269	285	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	LEU	conflict	UNP P66937
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
D	409	MET	LEU	conflict	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937
S	409	MET	LEU	conflict	UNP P66937
S	544	THR	-	linker	UNP P66937

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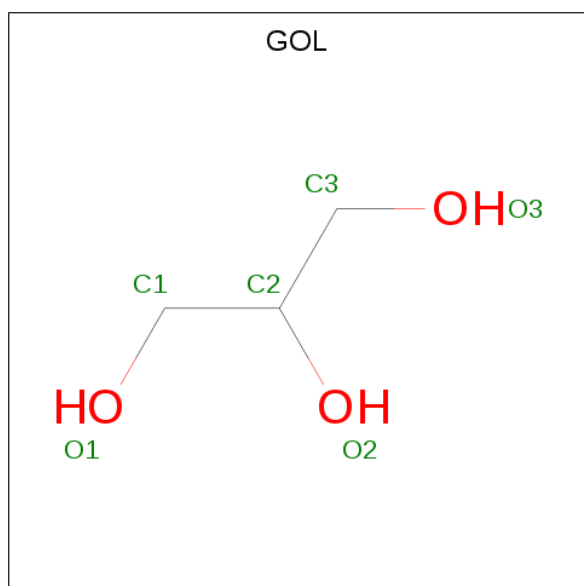
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Chain	Residue	Modelled	Actual	Comment	Reference
S	545	GLY	-	linker	UNP P66937
U	409	MET	LEU	conflict	UNP P66937
U	544	THR	-	linker	UNP P66937
U	545	GLY	-	linker	UNP P66937

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	P	0	0	0
			391	184	74	114	19			
3	F	20	Total	C	N	O	P	0	0	0
			391	184	74	114	19			
3	V	20	Total	C	N	O	P	0	0	0
			392	184	74	115	19			
3	W	20	Total	C	N	O	P	0	0	0
			393	186	74	114	19			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	T	1	Total	C	O	0	0
			6	3	3		
4	T	1	Total	C	O	0	0
			6	3	3		
4	U	1	Total	C	O	0	0
			6	3	3		
4	V	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	R	1	Total Na 1 1	0	0
6	T	1	Total Na 1 1	0	0

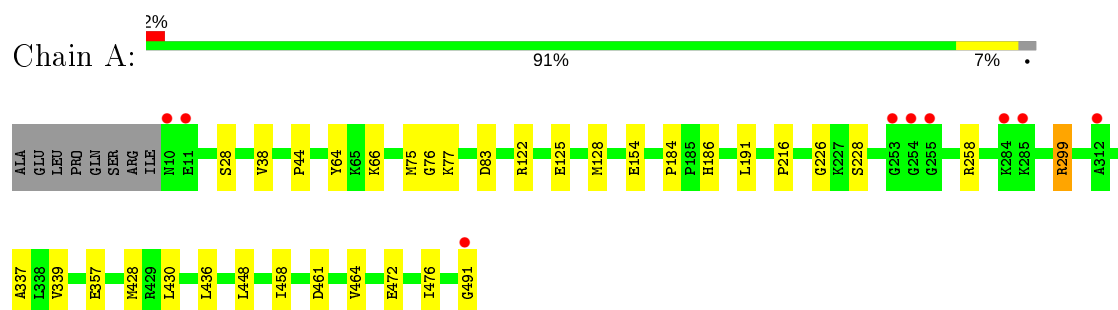
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	83	Total O 84 84	0	1
7	B	28	Total O 28 28	0	0
7	C	67	Total O 67 67	0	0
7	D	19	Total O 19 19	0	0
7	E	17	Total O 17 17	0	0
7	F	4	Total O 4 4	0	0
7	R	75	Total O 75 75	0	0
7	S	32	Total O 32 32	0	0
7	T	78	Total O 79 79	0	1
7	U	31	Total O 31 31	0	0
7	V	16	Total O 16 16	0	0
7	W	18	Total O 18 18	0	0

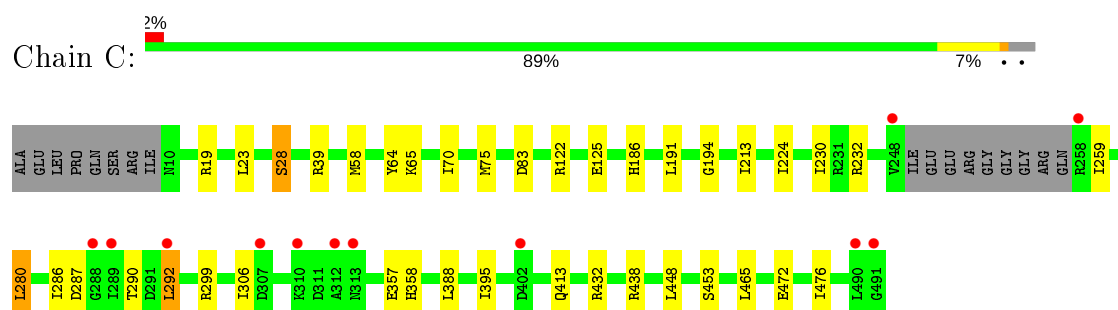
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

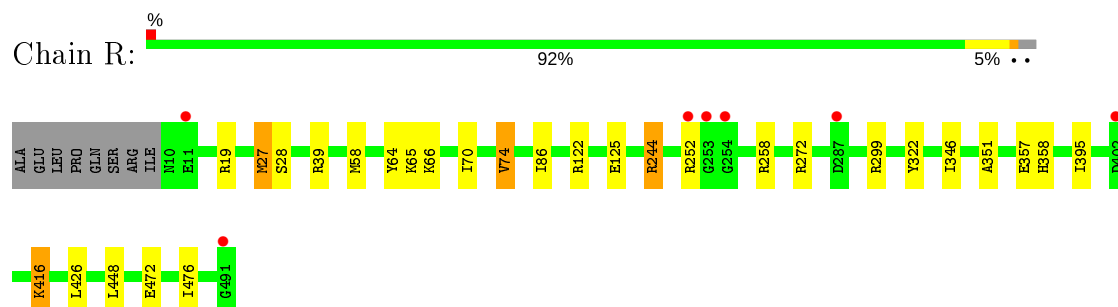
• Molecule 1: DNA gyrase subunit A



• Molecule 1: DNA gyrase subunit A

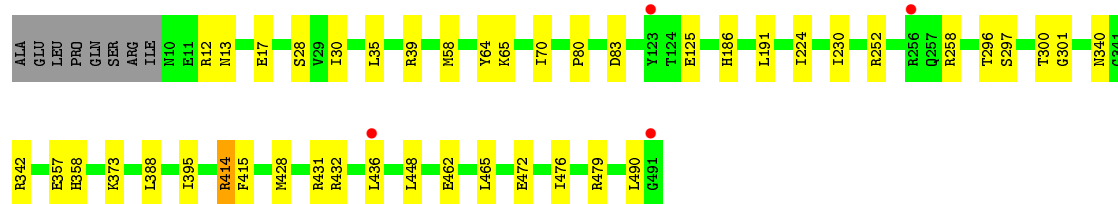


• Molecule 1: DNA gyrase subunit A

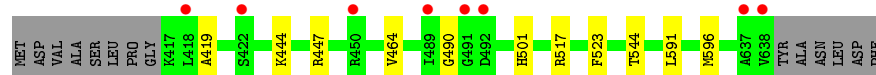
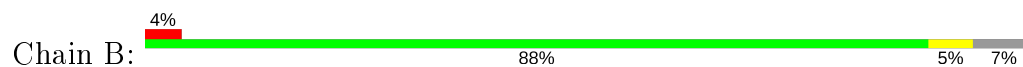


• Molecule 1: DNA gyrase subunit A

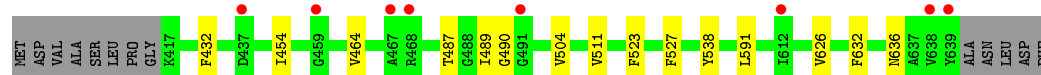
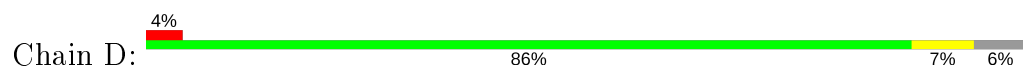




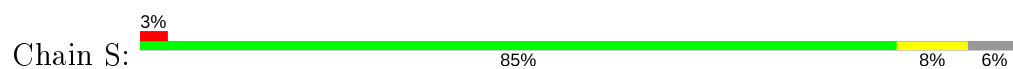
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



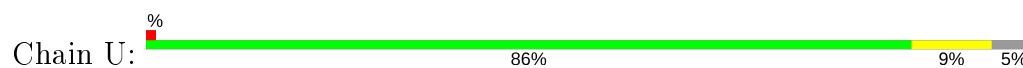
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



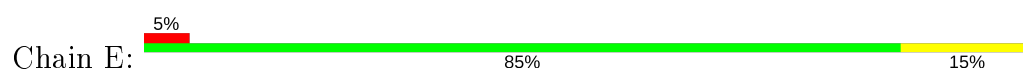
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



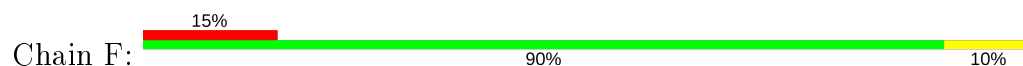
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

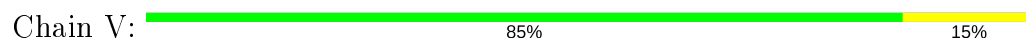


- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')





- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.28Å 124.64Å 155.24Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	19.91 – 2.60 19.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.91-2.60) 99.2 (19.91-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.236 0.206 , 0.242	Depositor DCC
R_{free} test set	5247 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23182	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	0.43	0/3884	0.63	1/5234 (0.0%)
1	C	0.43	0/3765	0.62	0/5083
1	R	0.44	0/3851	0.63	0/5198
1	T	0.44	0/3867	0.64	1/5215 (0.0%)
2	B	0.44	0/1479	0.67	0/2000
2	D	0.44	0/1449	0.68	0/1965
2	S	0.45	0/1522	0.65	0/2057
2	U	0.45	0/1538	0.67	0/2075
3	E	1.11	0/438	1.02	1/675 (0.1%)
3	F	1.14	0/438	1.01	0/675
3	V	1.13	0/439	1.06	1/677 (0.1%)
3	W	1.14	1/440 (0.2%)	1.11	2/678 (0.3%)
All	All	0.52	1/23110 (0.0%)	0.69	6/31532 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	5	DG	O5'-C5'	-5.33	1.28	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	8	DC	O4'-C4'-C3'	-6.12	102.05	104.50
3	W	8	DC	O4'-C4'-C3'	-5.61	102.25	104.50
3	W	5	DG	C4'-C3'-C2'	-5.49	98.16	103.10
1	A	76	GLY	N-CA-C	-5.46	99.46	113.10
3	V	8	DC	O4'-C4'-C3'	-5.38	102.35	104.50
1	T	300	THR	C-N-CA	5.18	133.19	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3833	0	3858	19	0
1	C	3718	0	3720	18	0
1	R	3803	0	3780	18	0
1	T	3819	0	3831	19	0
2	B	1456	0	1402	4	0
2	D	1426	0	1359	9	0
2	S	1498	0	1453	14	0
2	U	1514	0	1496	10	0
3	E	391	0	209	2	0
3	F	391	0	209	1	0
3	V	392	0	213	1	0
3	W	393	0	212	4	0
4	A	6	0	8	1	0
4	C	6	0	8	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	R	18	0	24	0	0
4	T	12	0	16	0	0
4	U	6	0	8	0	0
4	V	6	0	8	0	0
5	A	5	0	0	0	0
5	T	5	0	0	0	0
6	R	1	0	0	0	0
6	T	1	0	0	0	0
7	A	84	0	0	0	0
7	B	28	0	0	1	0
7	C	67	0	0	0	0
7	D	19	0	0	0	0
7	E	17	0	0	0	0
7	F	4	0	0	0	0
7	R	75	0	0	0	0
7	S	32	0	0	0	0
7	T	79	0	0	0	0
7	U	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	V	16	0	0	0	0
7	W	18	0	0	0	0
All	All	23182	0	21830	104	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 2.

All (104) 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)
2:D:489:ILE:HD12	2:D:527:PHE:HB3	1.60	0.83
2:S:443:THR:HG22	2:S:454:ILE:HG12	1.64	0.79
2:S:447:ARG:HD3	2:S:454:ILE:CD1	2.21	0.71
1:T:64:TYR:HB3	1:T:125:GLU:HB3	1.73	0.70
2:S:637:ALA:HB1	2:S:639[A]:TYR:CE2	2.26	0.69
1:R:64:TYR:HB3	1:R:125:GLU:HB3	1.74	0.69
2:S:447:ARG:HD3	2:S:454:ILE:HD11	1.74	0.69
2:U:447:ARG:HD3	2:U:454:ILE:CD1	2.23	0.68
1:R:27[A]:MET:CE	2:S:633:ILE:HG23	2.26	0.65
2:U:447:ARG:HD3	2:U:454:ILE:HD11	1.79	0.64
1:C:64:TYR:HB3	1:C:125:GLU:HB3	1.80	0.63
3:F:1:DG:H2''	3:F:2:DA:O5'	1.99	0.63
1:R:252:ARG:HD3	1:R:258:ARG:HB3	1.81	0.62
2:B:419:ALA:HB2	2:B:444:LYS:HE3	1.82	0.61
1:C:259:ILE:HD12	1:C:306:ILE:HD11	1.81	0.61
1:A:77:LYS:HB3	1:A:154:GLU:HG3	1.83	0.60
1:R:58:MET:HG2	1:R:65:LYS:HG3	1.84	0.60
1:R:122:ARG:HB3	1:T:80:PRO:HB2	1.83	0.59
2:U:419:ALA:HB2	2:U:444:LYS:HE3	1.84	0.59
2:U:505:ILE:HB	2:U:539:ILE:HD13	1.85	0.59
1:R:39:ARG:HB3	1:R:358:HIS:CD2	2.39	0.58
1:A:64:TYR:HB3	1:A:125:GLU:HB3	1.85	0.57
1:R:27[A]:MET:HE3	2:S:633:ILE:HG23	1.88	0.55
1:A:461:ASP:O	1:A:464:VAL:HG12	2.06	0.55
1:A:461:ASP:HB3	1:A:464:VAL:HG12	1.88	0.54
1:R:395:ILE:HD13	1:T:395:ILE:HD13	1.90	0.53
1:R:74:VAL:HG22	1:R:86:ILE:HG21	1.90	0.53
1:C:292:LEU:HB2	1:C:306:ILE:HG22	1.91	0.52
2:U:583:LEU:HD23	2:U:586:MET:CE	2.39	0.52
2:U:447:ARG:HD3	2:U:454:ILE:HD12	1.92	0.52
1:C:58:MET:SD	1:C:70:ILE:HG12	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:462:LEU:HD13	3:W:14:DT:H5''	1.93	0.51
1:R:27[A]:MET:HE1	2:S:633:ILE:HG23	1.93	0.51
1:T:58:MET:HG2	1:T:65:LYS:HG3	1.92	0.51
1:A:458:ILE:HA	1:A:464:VAL:HG13	1.93	0.51
2:U:460:LYS:HE3	7:U:823:HOH:O	2.10	0.51
1:R:58:MET:SD	1:R:70:ILE:HG12	2.51	0.50
1:T:428:MET:HG2	1:T:432[A]:ARG:HD3	1.94	0.50
1:T:12:ARG:HH11	1:T:17:GLU:HA	1.76	0.50
1:C:122:ARG:HH22	3:E:9:DG:P	2.34	0.50
1:A:226:GLY:HA2	1:A:491:GLY:HA3	1.94	0.50
2:D:432:PHE:HB2	2:D:454:ILE:HD13	1.94	0.50
2:U:464:VAL:HG21	2:U:523:PHE:HA	1.95	0.49
2:S:447:ARG:HD3	2:S:454:ILE:HD12	1.91	0.49
1:T:186:HIS:HB2	1:T:191:LEU:HD11	1.95	0.48
1:T:297:SER:O	1:T:301:GLY:HA2	2.14	0.48
1:A:38:VAL:HG11	1:A:339:VAL:HG22	1.94	0.48
1:C:19:ARG:HE	2:D:632:PHE:HE1	1.60	0.48
1:C:39:ARG:HB3	1:C:358:HIS:CD2	2.49	0.47
1:R:426:LEU:HB3	1:T:431:ARG:HB3	1.97	0.47
1:R:416:LYS:O	1:R:416:LYS:HG2	2.14	0.47
1:T:414:ARG:HD2	1:T:415:PHE:CZ	2.49	0.47
1:C:186:HIS:HB2	1:C:191:LEU:HD11	1.96	0.47
1:C:75:MET:SD	1:C:83:ASP:HB3	2.55	0.47
1:R:19:ARG:HE	2:S:632:PHE:HE1	1.63	0.47
1:T:39:ARG:HB3	1:T:358:HIS:CD2	2.50	0.47
1:A:75[A]:MET:SD	1:A:83:ASP:HB3	2.54	0.46
3:W:5:DG:H5'	3:W:5:DG:H2'	1.64	0.46
1:T:58:MET:SD	1:T:70:ILE:HG12	2.55	0.46
2:D:464:VAL:HG21	2:D:523:PHE:HA	1.97	0.46
1:T:252:ARG:HD3	1:T:258:ARG:HB3	1.96	0.46
1:R:66:LYS:HD2	1:R:122:ARG:O	2.16	0.46
1:A:38:VAL:HG12	1:A:337:ALA:HB3	1.98	0.45
2:B:517:ARG:HD3	7:B:716:HOH:O	2.15	0.45
2:S:581:LYS:HD2	2:S:581:LYS:HA	1.86	0.45
2:U:583:LEU:HD23	2:U:586:MET:HE1	1.97	0.45
1:R:244:ARG:HD2	1:R:322:TYR:CD1	2.51	0.45
2:S:464:VAL:HG21	2:S:523:PHE:HA	1.99	0.45
2:S:626:VAL:HG11	3:W:17:DG:H3'	1.97	0.45
1:A:184:PRO:HB2	1:A:216:PRO:HB3	2.00	0.44
2:D:626:VAL:HG11	3:E:17:DG:H3'	1.99	0.44
1:T:296:THR:HA	1:T:301:GLY:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:HD21	2:D:636:ASN:O	2.18	0.44
1:C:388:LEU:HD13	1:C:438:ARG:HD3	1.99	0.43
1:A:44:PRO:HB3	4:A:501:GOL:H31	1.99	0.43
2:S:464:VAL:HB	2:S:527:PHE:HE2	1.84	0.43
2:U:464:VAL:HB	2:U:527:PHE:HE2	1.84	0.43
1:C:280:LEU:HB3	1:C:286:ILE:HG22	2.01	0.43
1:A:38:VAL:CG1	1:A:337:ALA:HB3	2.50	0.42
1:A:430:LEU:HD22	1:C:395:ILE:HD13	2.00	0.42
1:C:472:GLU:O	1:C:476:ILE:HG12	2.19	0.42
1:R:472:GLU:O	1:R:476:ILE:HG12	2.19	0.42
2:D:464:VAL:HB	2:D:527:PHE:HE2	1.84	0.42
2:B:464:VAL:HG21	2:B:523:PHE:HA	2.01	0.42
1:C:58:MET:HG2	1:C:65:LYS:HD3	2.02	0.42
1:T:472:GLU:O	1:T:476:ILE:HG12	2.19	0.41
3:V:4:DC:H2'	3:V:5:DG:C8	2.55	0.41
1:C:224:ILE:HG21	1:C:230:ILE:HD11	2.02	0.41
1:C:28:SER:HB3	2:D:511:VAL:HG13	2.02	0.41
2:D:504:VAL:HG22	2:D:538:TYR:HB2	2.01	0.41
1:T:30:ILE:HG23	1:T:35:LEU:HD12	2.02	0.41
1:R:346:ILE:HD12	1:R:351:ALA:HB2	2.02	0.41
1:A:66:LYS:HD2	1:A:122:ARG:O	2.21	0.41
1:A:458:ILE:HA	1:A:464:VAL:CG1	2.51	0.41
1:C:194:GLY:HA3	1:C:213:ILE:HD11	2.02	0.41
1:A:128:MET:HB3	1:A:128:MET:HE3	1.90	0.41
1:T:224:ILE:HG21	1:T:230:ILE:HD11	2.02	0.41
1:T:373:LYS:HD3	1:T:373:LYS:HA	1.90	0.41
3:W:4:DC:H3'	3:W:5:DG:H5''	2.03	0.41
2:B:447:ARG:HB3	2:B:596:MET:HE1	2.03	0.40
1:A:186:HIS:HB2	1:A:191:LEU:HD11	2.03	0.40
1:T:12:ARG:HG2	1:T:13:ASN:H	1.86	0.40
1:A:472:GLU:O	1:A:476:ILE:HG12	2.21	0.40
1:A:299:ARG:H	1:A:299:ARG:HG2	1.50	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	486/490 (99%)	475 (98%)	11 (2%)	0	100	100
1	C	471/490 (96%)	460 (98%)	11 (2%)	0	100	100
1	R	485/490 (99%)	473 (98%)	12 (2%)	0	100	100
1	T	484/490 (99%)	469 (97%)	14 (3%)	1 (0%)	47	71
2	B	187/202 (93%)	181 (97%)	5 (3%)	1 (0%)	29	52
2	D	187/202 (93%)	180 (96%)	5 (3%)	2 (1%)	14	30
2	S	190/202 (94%)	181 (95%)	7 (4%)	2 (1%)	14	30
2	U	192/202 (95%)	185 (96%)	6 (3%)	1 (0%)	29	52
All	All	2682/2768 (97%)	2604 (97%)	71 (3%)	7 (0%)	47	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	490	GLY
2	S	638[A]	VAL
2	S	638[B]	VAL
2	D	487	THR
1	T	83	ASP
2	U	640	ALA
2	D	490	GLY

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	408/423 (96%)	400 (98%)	8 (2%)	55	78
1	C	396/423 (94%)	383 (97%)	13 (3%)	38	64
1	R	402/423 (95%)	392 (98%)	10 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	403/423 (95%)	391 (97%)	12 (3%)	41	67
2	B	149/168 (89%)	146 (98%)	3 (2%)	55	78
2	D	144/168 (86%)	143 (99%)	1 (1%)	84	94
2	S	154/168 (92%)	149 (97%)	5 (3%)	39	65
2	U	157/168 (94%)	151 (96%)	6 (4%)	33	59
All	All	2213/2364 (94%)	2155 (97%)	58 (3%)	46	72

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	228	SER
1	A	258	ARG
1	A	299	ARG
1	A	357	GLU
1	A	428	MET
1	A	436	LEU
1	A	448	LEU
2	B	501	HIS
2	B	544	THR
2	B	591	LEU
1	C	28	SER
1	C	232	ARG
1	C	280	LEU
1	C	287	ASP
1	C	290	THR
1	C	292	LEU
1	C	299	ARG
1	C	357	GLU
1	C	413	GLN
1	C	432	ARG
1	C	448	LEU
1	C	453	SER
1	C	465	LEU
2	D	591	LEU
1	R	27[A]	MET
1	R	27[B]	MET
1	R	28	SER
1	R	74	VAL
1	R	244	ARG

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Mol	Chain	Res	Type
1	R	272	ARG
1	R	299	ARG
1	R	357	GLU
1	R	416	LYS
1	R	448	LEU
2	S	501	HIS
2	S	544	THR
2	S	591	LEU
2	S	638[A]	VAL
2	S	638[B]	VAL
1	T	28	SER
1	T	340	ASN
1	T	342	ARG
1	T	357	GLU
1	T	388	LEU
1	T	414	ARG
1	T	436	LEU
1	T	448	LEU
1	T	462	GLU
1	T	465	LEU
1	T	479	ARG
1	T	490	LEU
2	U	477	GLU
2	U	489	ILE
2	U	529	ARG
2	U	544	THR
2	U	591	LEU
2	U	639	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	56	GLN
1	R	153	ASN
1	R	242	GLN
1	R	412	GLN
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 [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](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	F	101	-	5,5,5	0.04	0	5,5,5	0.20	0
4	GOL	R	501	-	5,5,5	0.09	0	5,5,5	0.22	0
4	GOL	R	503	-	5,5,5	0.08	0	5,5,5	0.31	0
4	GOL	C	501	-	5,5,5	0.05	0	5,5,5	0.38	0
4	GOL	E	101	-	5,5,5	0.08	0	5,5,5	0.18	0
4	GOL	T	502	-	5,5,5	0.07	0	5,5,5	0.23	0
4	GOL	R	502	-	5,5,5	0.11	0	5,5,5	0.36	0
4	GOL	T	501	-	5,5,5	0.15	0	5,5,5	0.29	0
4	GOL	U	701	-	5,5,5	0.13	0	5,5,5	0.31	0
4	GOL	V	101	-	5,5,5	0.07	0	5,5,5	0.28	0
4	GOL	A	501	-	5,5,5	0.08	0	5,5,5	0.26	0
5	SO4	T	503	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.12	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
4	GOL	F	101	-	-	0/4/4/4	-
4	GOL	R	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	501	-	-	2/4/4/4	-
4	GOL	E	101	-	-	0/4/4/4	-
4	GOL	T	502	-	-	0/4/4/4	-
4	GOL	R	502	-	-	0/4/4/4	-
4	GOL	T	501	-	-	0/4/4/4	-
4	GOL	U	701	-	-	0/4/4/4	-
4	GOL	R	501	-	-	0/4/4/4	-
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	V	101	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	GOL	O1-C1-C2-C3
4	C	501	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	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, 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	482/490 (98%)	-0.17	9 (1%) 66 62	40, 58, 90, 129	0
1	C	473/490 (96%)	-0.05	12 (2%) 57 51	39, 60, 104, 133	0
1	R	482/490 (98%)	-0.25	7 (1%) 73 70	34, 53, 96, 112	0
1	T	482/490 (98%)	-0.33	4 (0%) 86 84	31, 54, 85, 104	0
2	B	188/202 (93%)	0.22	8 (4%) 35 28	48, 72, 100, 124	0
2	D	189/202 (93%)	0.11	8 (4%) 36 29	49, 71, 109, 127	0
2	S	189/202 (93%)	-0.12	6 (3%) 47 40	41, 59, 83, 105	0
2	U	192/202 (95%)	-0.22	3 (1%) 72 68	40, 57, 87, 108	0
3	E	20/20 (100%)	0.17	1 (5%) 28 23	54, 69, 112, 120	0
3	F	20/20 (100%)	0.30	3 (15%) 2 1	56, 79, 110, 116	0
3	V	20/20 (100%)	-0.57	0 100 100	46, 57, 73, 78	0
3	W	20/20 (100%)	-0.57	0 100 100	47, 56, 71, 76	0
All	All	2757/2848 (96%)	-0.14	61 (2%) 62 56	31, 59, 97, 133	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	639[A]	TYR	8.9
1	C	491	GLY	7.2
2	U	639	TYR	5.4
1	A	254	GLY	5.2
2	S	638[A]	VAL	5.1
1	A	491	GLY	4.8
1	R	254	GLY	4.5
1	R	402[A]	ASP	4.4
2	B	492	ASP	4.1
3	F	1	DG	3.9
1	A	10	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	639	TYR	3.7
2	D	638	VAL	3.5
3	E	2	DA	3.4
1	C	307	ASP	3.4
2	D	459	GLY	3.2
1	A	11	GLU	3.2
1	T	436	LEU	3.1
1	C	312	ALA	3.1
1	C	288	GLY	3.0
1	A	253	GLY	3.0
2	D	468	ARG	3.0
2	B	638	VAL	2.9
2	B	489	ILE	2.8
2	B	491	GLY	2.7
1	C	258	ARG	2.6
1	R	253	GLY	2.5
1	R	287	ASP	2.5
1	C	292	LEU	2.5
2	S	589	ASP	2.5
1	C	248	VAL	2.5
2	U	638	VAL	2.5
1	A	255	GLY	2.5
1	C	289	ILE	2.5
2	B	422	SER	2.5
2	D	491	GLY	2.4
2	B	418	LEU	2.4
1	C	313	ASN	2.4
2	D	612	ILE	2.4
2	S	491	GLY	2.4
1	A	284	LYS	2.4
2	B	450[A]	ARG	2.4
2	S	545	GLY	2.3
3	F	2	DA	2.3
1	R	491	GLY	2.3
2	D	467	ALA	2.3
2	B	637	ALA	2.3
1	A	285	LYS	2.3
1	T	123	TYR	2.2
3	F	20	DT	2.2
1	C	310	LYS	2.1
2	S	612	ILE	2.1
1	R	11	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	T	491	GLY	2.1
1	T	256	ARG	2.1
1	R	252	ARG	2.1
1	C	402	ASP	2.0
1	A	312	ALA	2.0
2	D	437	ASP	2.0
2	U	624	ASP	2.0
1	C	490	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
4	GOL	R	503	6/6	0.65	0.32	92,94,96,97	0
4	GOL	T	502	6/6	0.65	0.34	102,104,104,104	0
4	GOL	V	101	6/6	0.77	0.39	93,94,96,96	0
4	GOL	U	701	6/6	0.84	0.17	63,64,65,66	0
4	GOL	R	502	6/6	0.85	0.30	71,75,77,78	0
6	NA	T	504	1/1	0.89	0.14	65,65,65,65	0
4	GOL	E	101	6/6	0.89	0.24	71,73,74,74	0
4	GOL	A	501	6/6	0.90	0.20	62,70,72,72	0
4	GOL	F	101	6/6	0.90	0.19	82,86,87,88	0
4	GOL	R	501	6/6	0.91	0.18	44,51,53,55	0
4	GOL	C	501	6/6	0.92	0.26	60,66,68,70	0
6	NA	R	504	1/1	0.93	0.06	66,66,66,66	0
4	GOL	T	501	6/6	0.93	0.14	48,57,61,62	0
5	SO4	A	502	5/5	0.93	0.22	110,111,111,111	0
5	SO4	T	503	5/5	0.95	0.18	136,137,137,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.