



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:46 AM UTC

PDB ID : 1TK5 / pdb_00001tk5
Title : T7 DNA polymerase binary complex with 8 oxo guanosine in the templating strand
Authors : Brieba, L.G.; Eichman, B.F.; Kokoska, R.J.; Doublet, S.; Kunkel, T.A.; Ellenberger, T.
Deposited on : 2004-06-08
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

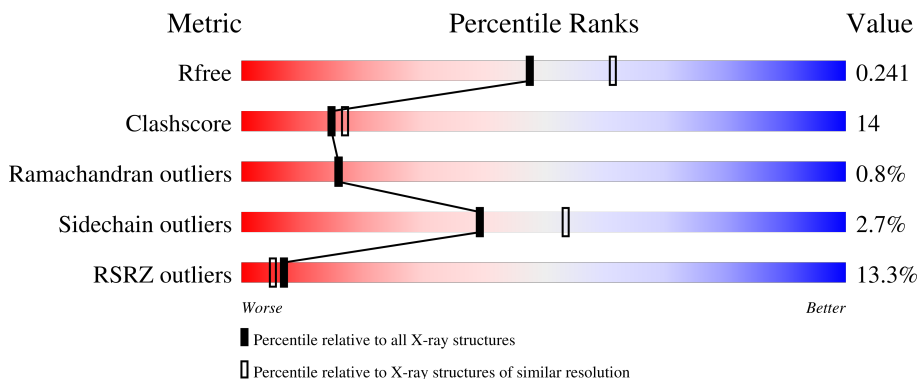
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of 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	P	22	
2	T	26	
3	A	698	
4	B	108	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7441 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*CP*GP*AP*AP*A*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG)P*TP*GP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	11	222	106	44	62	10	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(8OG)P*CP*TP*GP*GP*CP*AP*C P*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	13	266	125	49	79	13	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	681	5340	3405	923	988	24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P00581
A	?	-	ARG	deletion	UNP P00581
A	?	-	PHE	deletion	UNP P00581
A	?	-	GLY	deletion	UNP P00581
A	?	-	SER	deletion	UNP P00581
A	?	-	HIS	deletion	UNP P00581

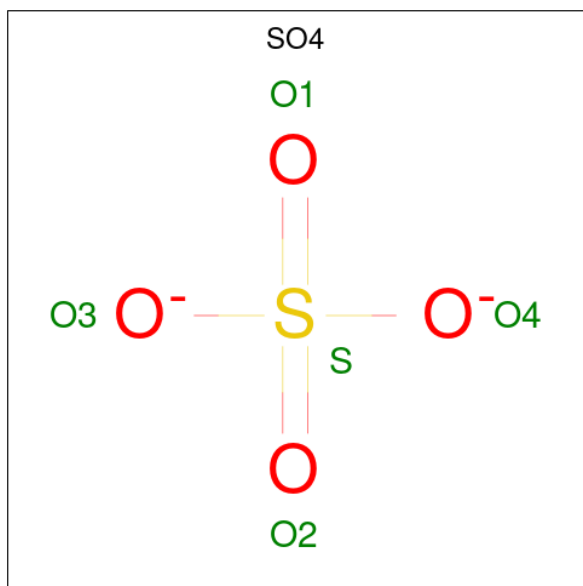
- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	105	802	518	129	152	3	0	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

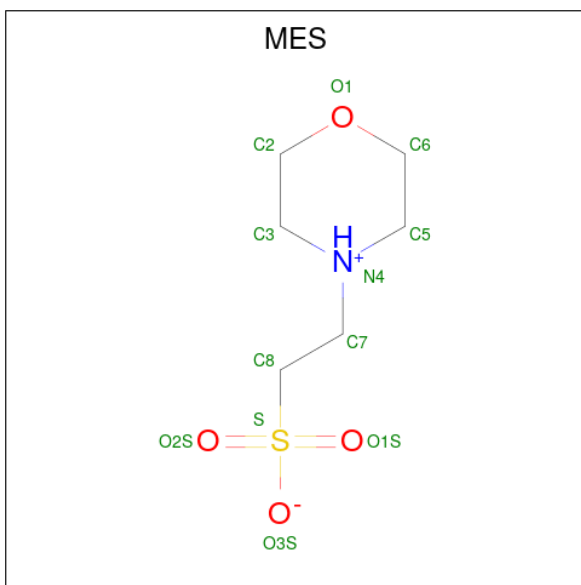
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



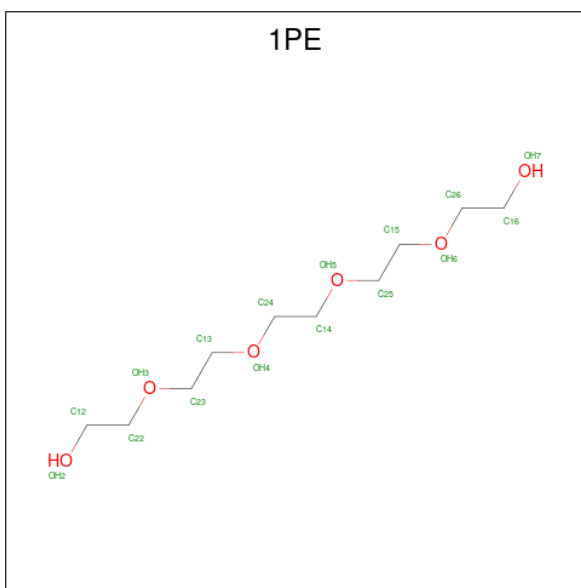
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	A	1	12	6	1	4	1	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	16	10	6	0	0

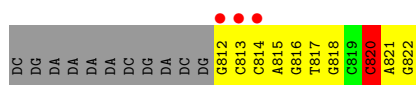
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	P	27	Total O 27 27	0	0
9	T	48	Total O 48 48	0	0
9	A	649	Total O 649 649	0	0
9	B	48	Total O 48 48	0	0

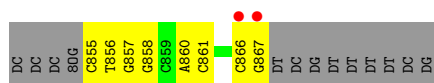
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

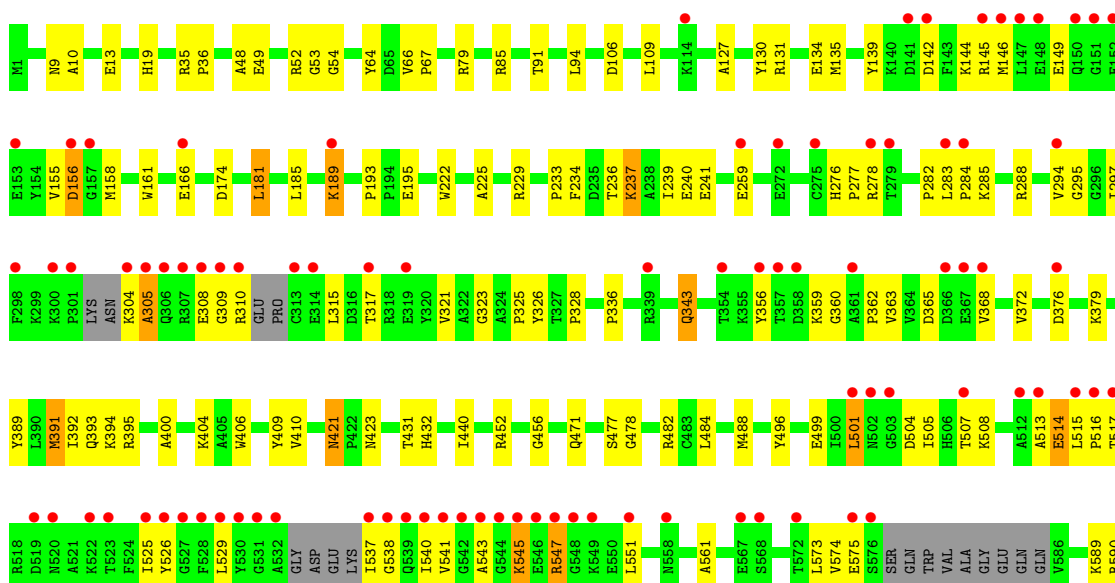
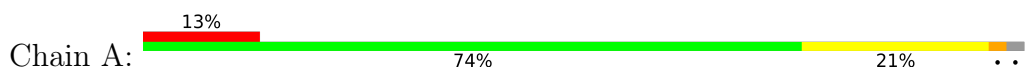
- Molecule 1: 5'-D(*CP*GP*AP*AP*A*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG)P*T P*GP*CP*AP*A)-3'



- Molecule 2: 5'-D(*CP*CP*CP*(8OG)P*CP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*G P*TP*CP*GP*TP*TP*TP*TP*CP*G)-3'

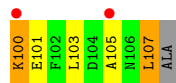
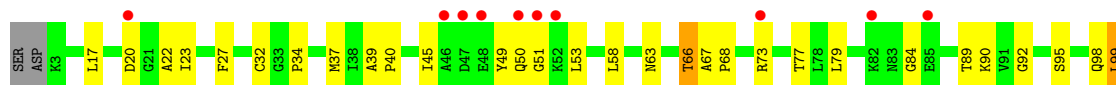


- Molecule 3: DNA polymerase





● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.31Å 213.26Å 52.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.33 – 2.20 26.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (26.33-2.20) 99.5 (26.33-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 1.99Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.246 0.209 , 0.241	Depositor DCC
R_{free} test set	3873 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7441	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 1PE, MG, SO4, DDG

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	P	0.29	0/225	0.86	2/345 (0.6%)
2	T	0.33	0/297	0.79	0/456
3	A	0.39	0/5470	0.85	9/7413 (0.1%)
4	B	0.34	0/817	0.84	3/1108 (0.3%)
All	All	0.38	0/6809	0.85	14/9322 (0.2%)

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	P	0	1
2	T	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	127	ALA	N-CA-C	8.06	119.69	111.07
3	A	589	LYS	N-CA-C	-7.99	104.05	113.88
4	B	66	THR	N-CA-C	7.75	119.51	111.14
3	A	400	ALA	N-CA-C	6.36	121.64	113.18
3	A	225	ALA	N-CA-C	-5.91	104.92	111.36
4	B	63	ASN	CA-C-N	5.82	125.92	119.87
4	B	63	ASN	C-N-CA	5.82	125.92	119.87
3	A	9	ASN	N-CA-C	5.80	120.22	113.20
1	P	820	DC	C4'-C3'-O3'	5.19	117.78	110.00
3	A	421	ASN	N-CA-C	-5.09	98.61	108.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	309	GLY	N-CA-C	-5.07	108.77	114.40
1	P	820	DC	N1-C1'-C2'	-5.03	105.96	113.50
3	A	283	LEU	CA-C-N	5.01	125.03	119.32
3	A	283	LEU	C-N-CA	5.01	125.03	119.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	820	DC	Sidechain
2	T	857	DG	Sidechain

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	P	222	0	124	23	0
2	T	266	0	146	7	0
3	A	5340	0	5156	135	0
4	B	802	0	816	22	0
5	A	1	0	0	0	0
6	A	10	0	0	0	0
7	A	12	0	13	0	0
8	A	16	0	22	1	0
9	A	649	0	0	8	0
9	B	48	0	0	0	0
9	P	27	0	0	0	0
9	T	48	0	0	1	0
All	All	7441	0	6277	179	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 14.

All (179) 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:P:815:DA:H2''	1:P:816:DG:H5'	1.39	1.04
3:A:537:ILE:HG13	3:A:538:GLY:H	1.27	0.97
1:P:820:DC:H2''	1:P:821:DA:H5'	1.49	0.93
1:P:817:DT:H2''	1:P:818:DG:H5'	1.53	0.91
1:P:820:DC:H2''	1:P:821:DA:C5'	2.03	0.88
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.55	0.86
3:A:391:MET:C	3:A:391:MET:HE2	2.09	0.78
1:P:816:DG:H2''	1:P:817:DT:C5'	2.13	0.78
2:T:866:DC:H2''	2:T:867:DG:C8	2.19	0.76
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.67	0.75
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.15	0.75
1:P:812:DG:H2'	1:P:813:DC:H5''	1.69	0.74
3:A:391:MET:HE3	3:A:395:ARG:HG3	1.69	0.74
3:A:285:LYS:HA	3:A:285:LYS:HE2	1.68	0.73
3:A:537:ILE:HG13	3:A:538:GLY:N	2.03	0.72
3:A:391:MET:HE2	3:A:392:ILE:HA	1.71	0.72
1:P:816:DG:H2''	1:P:817:DT:H5''	1.72	0.71
3:A:391:MET:HE3	3:A:395:ARG:CG	2.21	0.71
3:A:145:ARG:O	3:A:149:GLU:HG3	1.92	0.70
3:A:504:ASP:OD2	3:A:507:THR:HG23	1.90	0.70
3:A:547:ARG:O	3:A:547:ARG:HD3	1.91	0.70
3:A:632:MET:HA	3:A:635:GLU:HG2	1.73	0.70
3:A:667:GLN:HG2	3:A:696:MET:HE1	1.74	0.69
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.73	0.68
4:B:95:SER:OG	4:B:98:GLN:HG3	1.94	0.68
1:P:815:DA:C2'	1:P:816:DG:H5'	2.23	0.67
3:A:376:ASP:OD2	3:A:379:LYS:HG3	1.97	0.65
1:P:821:DA:H5'	1:P:821:DA:H8	1.61	0.65
4:B:77:THR:HG22	4:B:79:LEU:HD13	1.80	0.64
1:P:816:DG:C2'	1:P:817:DT:H5''	2.28	0.63
1:P:816:DG:H2''	1:P:817:DT:H5'	1.81	0.63
3:A:391:MET:HE2	3:A:392:ILE:N	2.14	0.62
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.81	0.62
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.40	0.62
3:A:66:VAL:HB	3:A:67:PRO:HD3	1.80	0.61
2:T:860:DA:H2''	2:T:861:DC:H5'	1.82	0.61
3:A:484:LEU:O	3:A:488:MET:HG2	2.01	0.61
2:T:855:DC:H2''	2:T:856:DT:H5'	1.82	0.61
1:P:817:DT:H2''	1:P:818:DG:C5'	2.28	0.60
3:A:391:MET:HE2	3:A:392:ILE:CA	2.30	0.60
4:B:100:LYS:NZ	4:B:100:LYS:HB3	2.17	0.60
3:A:525:ILE:HG23	3:A:526:TYR:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:499:GLU:HG2	3:A:508:LYS:HD2	1.84	0.60
3:A:156:ASP:HB2	9:A:1366:HOH:O	2.01	0.60
1:P:814:DC:H2''	1:P:815:DA:H5''	1.85	0.59
3:A:135:MET:HG3	3:A:174:ASP:OD1	2.03	0.59
3:A:667:GLN:O	3:A:671:GLU:HG3	2.03	0.59
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.84	0.59
3:A:321:VAL:HG23	4:B:90:LYS:HD2	1.84	0.58
3:A:308:GLU:C	3:A:310:ARG:H	2.10	0.58
3:A:574:VAL:HG12	3:A:575:GLU:N	2.19	0.58
1:P:812:DG:C2'	1:P:813:DC:H5''	2.32	0.58
3:A:135:MET:HA	3:A:135:MET:HE2	1.86	0.58
3:A:504:ASP:HB3	3:A:507:THR:OG1	2.04	0.58
3:A:663:GLU:HG2	3:A:696:MET:SD	2.44	0.58
3:A:236:THR:O	3:A:240:GLU:HG3	2.04	0.57
3:A:336:PRO:HB2	3:A:389:TYR:CD1	2.40	0.56
3:A:155:VAL:HG12	9:A:1366:HOH:O	2.05	0.56
3:A:234:PHE:CD2	3:A:410:VAL:HG11	2.41	0.56
3:A:229:ARG:HD2	9:A:1039:HOH:O	2.06	0.56
3:A:597:ASP:OD1	3:A:599:ARG:CD	2.54	0.55
3:A:49:GLU:OE2	3:A:54:GLY:HA3	2.07	0.55
3:A:496:TYR:CE1	3:A:505:ILE:HD11	2.42	0.54
3:A:304:LYS:O	3:A:305:ALA:HB2	2.06	0.54
3:A:19:HIS:O	3:A:36:PRO:HD3	2.06	0.54
1:P:815:DA:H2''	1:P:816:DG:C5'	2.27	0.54
3:A:142:ASP:O	3:A:146:MET:HG3	2.08	0.54
3:A:237:LYS:O	3:A:237:LYS:HD3	2.08	0.54
3:A:308:GLU:C	3:A:310:ARG:N	2.65	0.53
3:A:64:TYR:O	3:A:67:PRO:HD2	2.08	0.53
3:A:488:MET:HE2	3:A:496:TYR:HB2	1.90	0.53
3:A:496:TYR:CZ	3:A:505:ILE:HD11	2.44	0.53
3:A:131:ARG:O	3:A:135:MET:HG2	2.09	0.53
3:A:297:ILE:CD1	4:B:101:GLU:HB2	2.38	0.53
3:A:276:HIS:CD2	3:A:278:ARG:H	2.27	0.52
3:A:501:LEU:HD21	9:A:1535:HOH:O	2.09	0.52
4:B:37:MET:O	4:B:40:PRO:HD2	2.10	0.51
3:A:513:ALA:O	3:A:514:GLU:C	2.53	0.51
1:P:821:DA:H5'	1:P:821:DA:C8	2.44	0.51
3:A:106:ASP:OD2	3:A:109:LEU:HD12	2.10	0.51
3:A:195:GLU:H	3:A:195:GLU:CD	2.18	0.51
3:A:79:ARG:HD3	9:A:1127:HOH:O	2.11	0.51
3:A:391:MET:CE	3:A:395:ARG:HG3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:237:LYS:HD3	3:A:237:LYS:C	2.35	0.51
1:P:814:DC:H2''	1:P:815:DA:C5'	2.41	0.50
1:P:816:DG:H1'	1:P:817:DT:H5''	1.93	0.50
1:P:820:DC:H2''	1:P:821:DA:H5''	1.89	0.50
3:A:284:PRO:HA	3:A:288:ARG:NH2	2.27	0.50
3:A:189:LYS:HD3	3:A:189:LYS:C	2.38	0.49
3:A:478:GLY:O	3:A:482:ARG:HG3	2.12	0.49
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.93	0.49
3:A:391:MET:HE2	3:A:391:MET:O	2.12	0.49
4:B:58:LEU:HD21	4:B:66:THR:HB	1.93	0.49
1:P:814:DC:C2'	1:P:815:DA:H5''	2.43	0.49
3:A:499:GLU:HG2	3:A:508:LYS:CD	2.42	0.48
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.49	0.48
3:A:297:ILE:HD13	4:B:101:GLU:HB2	1.94	0.48
3:A:391:MET:HE3	3:A:395:ARG:HG2	1.93	0.48
2:T:858:DG:H4'	3:A:432:HIS:O	2.13	0.48
3:A:667:GLN:CG	3:A:696:MET:HE1	2.43	0.48
3:A:323:GLY:O	3:A:325:PRO:HD3	2.14	0.48
3:A:49:GLU:HA	3:A:52:ARG:HH11	1.79	0.48
3:A:139:TYR:HE1	3:A:166:GLU:HG3	1.79	0.48
3:A:365:ASP:O	3:A:368:VAL:HG22	2.14	0.48
3:A:440:ILE:O	3:A:452:ARG:NH1	2.47	0.48
3:A:233:PRO:HB2	3:A:456:GLY:O	2.14	0.47
3:A:488:MET:HE3	3:A:561:ALA:HB3	1.95	0.47
3:A:599:ARG:HD3	3:A:620:LEU:HD11	1.97	0.47
3:A:537:ILE:CD1	3:A:545:LYS:H	2.28	0.47
1:P:817:DT:OP1	3:A:359:LYS:HB3	2.14	0.47
3:A:155:VAL:O	3:A:156:ASP:C	2.57	0.47
3:A:574:VAL:CG1	3:A:575:GLU:N	2.78	0.47
3:A:678:ARG:NH2	3:A:689:LEU:HD21	2.29	0.47
1:P:821:DA:H2'	1:P:822:DDG:C8	2.44	0.46
3:A:541:VAL:HG23	3:A:543:ALA:H	1.80	0.46
3:A:237:LYS:O	3:A:241:GLU:HG3	2.15	0.46
3:A:91:THR:HB	3:A:181:LEU:HD13	1.97	0.46
3:A:48:ALA:O	3:A:52:ARG:HG3	2.15	0.46
3:A:193:PRO:HG3	9:A:1232:HOH:O	2.15	0.46
3:A:356:TYR:HD2	3:A:360:GLY:O	1.99	0.46
3:A:130:TYR:CZ	3:A:134:GLU:HG3	2.50	0.46
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.15	0.46
3:A:234:PHE:CD2	3:A:410:VAL:CG1	2.99	0.45
3:A:368:VAL:O	3:A:372:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:516:PRO:HG2	3:A:517:THR:H	1.81	0.45
3:A:666:ALA:HB3	3:A:696:MET:HE2	1.98	0.45
3:A:282:PRO:C	3:A:284:PRO:HD3	2.41	0.45
3:A:638:LEU:CD1	3:A:638:LEU:N	2.80	0.45
3:A:328:PRO:HB3	4:B:73:ARG:HH12	1.82	0.44
3:A:529:LEU:O	3:A:611:ASN:HB2	2.17	0.44
3:A:158:MET:HA	3:A:161:TRP:CE2	2.51	0.44
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.53	0.44
3:A:513:ALA:O	3:A:515:LEU:HG	2.17	0.44
3:A:525:ILE:CG2	3:A:526:TYR:N	2.79	0.44
3:A:538:GLY:C	3:A:540:ILE:H	2.25	0.44
1:P:821:DA:H2'	1:P:822:DDG:H8	2.00	0.43
3:A:525:ILE:HG23	3:A:526:TYR:H	1.81	0.43
3:A:638:LEU:N	3:A:638:LEU:HD12	2.33	0.43
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.82	0.43
3:A:10:ALA:C	8:A:992:1PE:H251	2.44	0.43
3:A:406:TRP:O	3:A:410:VAL:HG13	2.18	0.43
3:A:597:ASP:OD1	3:A:599:ARG:HD3	2.19	0.43
3:A:49:GLU:HA	3:A:52:ARG:NH1	2.34	0.43
4:B:103:LEU:O	4:B:107:LEU:HD22	2.18	0.43
4:B:49:TYR:HB3	4:B:53:LEU:HB3	2.00	0.43
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.19	0.43
2:T:860:DA:H2''	2:T:861:DC:C5'	2.48	0.42
3:A:391:MET:CE	3:A:392:ILE:HA	2.43	0.42
3:A:590:ARG:HD3	3:A:592:TRP:CE2	2.55	0.42
3:A:666:ALA:CB	3:A:696:MET:HE2	2.49	0.42
3:A:13:GLU:H	3:A:13:GLU:CD	2.27	0.42
2:T:856:DT:H2'	9:T:1070:HOH:O	2.20	0.42
3:A:573:LEU:HD21	3:A:593:ILE:CD1	2.49	0.42
3:A:590:ARG:HD2	3:A:592:TRP:O	2.19	0.42
3:A:452:ARG:HG3	3:A:700:TRP:HB3	2.01	0.42
4:B:27:PHE:CE1	4:B:79:LEU:HD22	2.55	0.42
3:A:538:GLY:C	3:A:540:ILE:N	2.78	0.42
4:B:17:LEU:HA	4:B:84:GLY:HA2	2.02	0.42
4:B:22:ALA:O	4:B:23:ILE:HD13	2.20	0.42
3:A:505:ILE:HD12	3:A:508:LYS:HD3	2.02	0.41
3:A:547:ARG:HD3	3:A:547:ARG:C	2.43	0.41
3:A:363:VAL:O	3:A:368:VAL:HG21	2.20	0.41
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.20	0.41
3:A:477:SER:O	3:A:478:GLY:C	2.64	0.41
3:A:674:GLN:NE2	3:A:678:ARG:HH11	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:317:THR:O	3:A:317:THR:HG22	2.20	0.41
3:A:547:ARG:CD	3:A:551:LEU:HG	2.51	0.41
4:B:49:TYR:C	4:B:51:GLY:N	2.79	0.41
2:T:855:DC:C2'	2:T:856:DT:H5'	2.48	0.41
3:A:326:TYR:HB3	4:B:92:GLY:HA2	2.03	0.41
4:B:67:ALA:HB3	4:B:68:PRO:HD3	2.01	0.41
3:A:53:GLY:HA2	9:A:1095:HOH:O	2.20	0.41
3:A:394:LYS:HA	3:A:394:LYS:HD3	1.91	0.41
3:A:423:ASN:OD1	3:A:599:ARG:NH2	2.53	0.41
3:A:294:VAL:HG12	3:A:295:GLY:N	2.36	0.40
3:A:144:LYS:HE2	3:A:144:LYS:HB3	1.88	0.40
4:B:49:TYR:C	4:B:51:GLY:H	2.29	0.40
3:A:452:ARG:NH2	9:A:1716:HOH:O	2.48	0.40
3:A:276:HIS:HD2	3:A:277:PRO:HD2	1.86	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	
3	A	671/698 (96%)	643 (96%)	23 (3%)	5 (1%)	18	19
4	B	103/108 (95%)	99 (96%)	3 (3%)	1 (1%)	12	11
All	All	774/806 (96%)	742 (96%)	26 (3%)	6 (1%)	16	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	305	ALA
3	A	545	LYS
3	A	653	HIS

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Mol	Chain	Res	Type
4	B	50	GLN
3	A	514	GLU

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	
3	A	542/579 (94%)	530 (98%)	12 (2%)	45	61
4	B	85/87 (98%)	80 (94%)	5 (6%)	18	22
All	All	627/666 (94%)	610 (97%)	17 (3%)	39	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	181	LEU
3	A	189	LYS
3	A	237	LYS
3	A	259	GLU
3	A	343	GLN
3	A	391	MET
3	A	393	GLN
3	A	501	LEU
3	A	547	ARG
3	A	599	ARG
3	A	624	LEU
3	A	686	PHE
4	B	20	ASP
4	B	89	THR
4	B	99	LEU
4	B	100	LYS
4	B	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	227	GLN
3	A	276	HIS
3	A	343	GLN
3	A	347	GLN
3	A	510	GLN
4	B	50	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	DDG	P	822	2,1	20,23,24	0.37	0	27,33,36	0.43	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
1	DDG	P	822	2,1	-	0/7/18/19	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	822	DDG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	SO4	A	905	-	4,4,4	0.37	0	6,6,6	0.11	0
8	1PE	A	992	-	15,15,15	0.90	0	14,14,14	0.94	0
6	SO4	A	904	-	4,4,4	0.33	0	6,6,6	0.08	0
7	MES	A	991	-	12,12,12	0.56	0	15,16,16	0.68	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
8	1PE	A	992	-	-	4/13/13/13	-
7	MES	A	991	-	-	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	991	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
7	A	991	MES	C7-C8-S-O3S
7	A	991	MES	C7-C8-S-O2S
8	A	992	1PE	C13-C23-OH3-C22
8	A	992	1PE	C25-C15-OH6-C26
8	A	992	1PE	OH2-C12-C22-OH3
8	A	992	1PE	OH4-C13-C23-OH3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	992	1PE	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	P	10/22 (45%)	1.19	3 (30%) 1 1	25, 40, 96, 97	0
2	T	13/26 (50%)	0.55	2 (15%) 5 4	20, 35, 95, 99	0
3	A	681/698 (97%)	0.39	91 (13%) 7 5	11, 26, 69, 89	0
4	B	105/108 (97%)	0.64	12 (11%) 10 7	21, 36, 53, 59	0
All	All	809/854 (94%)	0.43	108 (13%) 7 5	11, 27, 69, 99	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	548	GLY	8.1
3	A	156	ASP	5.9
3	A	537	ILE	5.7
3	A	538	GLY	5.6
3	A	301	PRO	5.5
3	A	278	ARG	5.4
3	A	308	GLU	5.1
3	A	546	GLU	5.1
3	A	507	THR	4.8
3	A	306	GLN	4.4
3	A	313	CYS	4.4
3	A	513	ALA	4.3
3	A	530	TYR	4.2
3	A	151	GLY	4.2
3	A	544	GLY	4.0
3	A	502	ASN	4.0
3	A	520	ASN	4.0
3	A	539	GLN	3.9
3	A	540	ILE	3.8
3	A	166	GLU	3.8
3	A	279	THR	3.7

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Mol	Chain	Res	Type	RSRZ
3	A	358	ASP	3.7
3	A	503	GLY	3.6
3	A	146	MET	3.6
3	A	309	GLY	3.6
3	A	541	VAL	3.6
3	A	545	LYS	3.6
3	A	305	ALA	3.6
3	A	543	ALA	3.6
2	T	866	DC	3.5
3	A	515	LEU	3.4
4	B	47	ASP	3.4
3	A	531	GLY	3.3
3	A	145	ARG	3.3
3	A	704	HIS	3.3
3	A	525	ILE	3.2
3	A	526	TYR	3.1
3	A	307	ARG	3.0
3	A	189	LYS	3.0
3	A	549	LYS	3.0
3	A	157	GLY	3.0
1	P	813	DC	3.0
1	P	814	DC	3.0
3	A	532	ALA	3.0
3	A	527	GLY	3.0
3	A	575	GLU	3.0
3	A	547	ARG	3.0
2	T	867	DG	2.9
4	B	82	LYS	2.9
3	A	529	LEU	2.9
3	A	314	GLU	2.9
3	A	516	PRO	2.9
3	A	501	LEU	2.8
1	P	812	DG	2.8
3	A	142	ASP	2.8
3	A	147	LEU	2.8
3	A	298	PHE	2.8
3	A	517	THR	2.7
3	A	523	THR	2.7
3	A	576	SER	2.7
3	A	693	GLU	2.7
3	A	512	ALA	2.7
3	A	150	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
4	B	50	GLN	2.6
3	A	522	LYS	2.6
3	A	294	VAL	2.6
3	A	357	THR	2.5
3	A	259	GLU	2.5
4	B	73	ARG	2.5
3	A	304	LYS	2.5
3	A	356	TYR	2.5
4	B	20	ASP	2.5
3	A	319	GLU	2.4
3	A	558	ASN	2.4
3	A	542	GLY	2.3
4	B	85	GLU	2.3
4	B	52	LYS	2.3
3	A	317	THR	2.3
3	A	572	THR	2.3
3	A	148	GLU	2.3
3	A	283	LEU	2.3
3	A	284	PRO	2.3
3	A	361	ALA	2.3
3	A	568	SER	2.3
3	A	152	GLU	2.3
3	A	300	LYS	2.3
3	A	275	CYS	2.2
3	A	153	GLU	2.2
3	A	367	GLU	2.2
4	B	51	GLY	2.2
3	A	605	SER	2.2
3	A	354	THR	2.2
3	A	310	ARG	2.2
3	A	551	LEU	2.2
3	A	528	PHE	2.2
3	A	339	ARG	2.1
3	A	272	GLU	2.1
3	A	567	GLU	2.1
4	B	48	GLU	2.1
3	A	366	ASP	2.1
3	A	376	ASP	2.1
3	A	368	VAL	2.1
3	A	114	LYS	2.1
3	A	519	ASP	2.1
4	B	46	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	141	ASP	2.0
4	B	105	ALA	2.0
4	B	100	LYS	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. 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
1	DDG	P	822	21/22	0.96	0.08	22,25,26,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	SO4	A	905	5/5	0.81	0.16	77,77,78,78	0
8	1PE	A	992	16/16	0.85	0.16	45,51,60,62	0
6	SO4	A	904	5/5	0.86	0.17	74,74,76,76	0
7	MES	A	991	12/12	0.93	0.10	39,41,45,45	0
5	MG	A	903	1/1	0.98	0.07	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.