Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:25 PM GMT

PDB ID	:	3TW4
Title	:	Crystal Structure of Human Septin 7 GTPase Domain
Authors	:	Serrao, V.H.B.; Alessandro, F.; Pereira, H.M.; Thiemann, O.T; Garratt, R.C.
Deposited on	:	2011-09-21
Resolution	:	3.35 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:

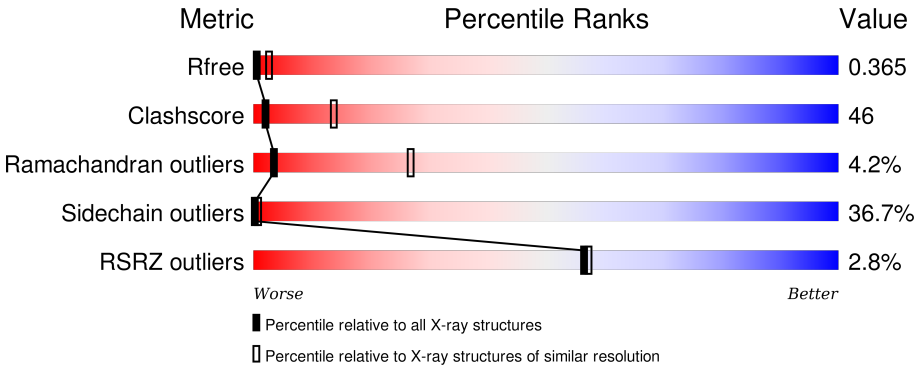
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	271	% 32% 32% 15% • 20%
1	B	271	3% 28% 32% 17% • 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GDP	A	500	-	-	X	-
2	GDP	B	501	-	-	X	-

2 Entry composition

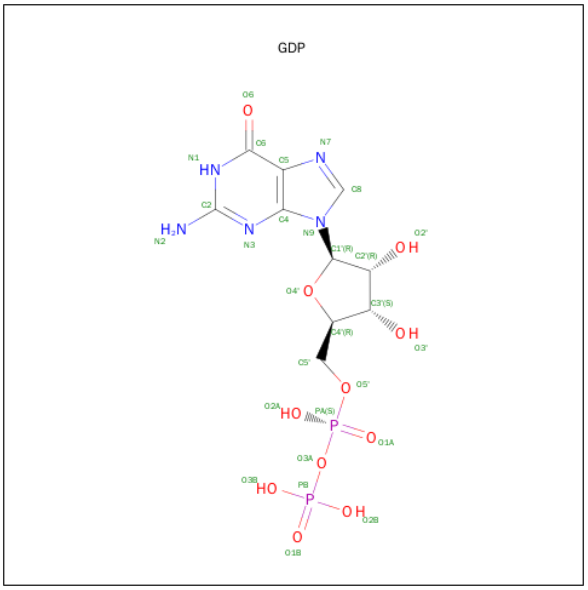
There are 2 unique types of molecules in this entry. The entry contains 3039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Septin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	10	0	0
			1512	955	260	289	8			
1	B	212	Total	C	N	O	S	10	0	0
			1471	943	250	271	7			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



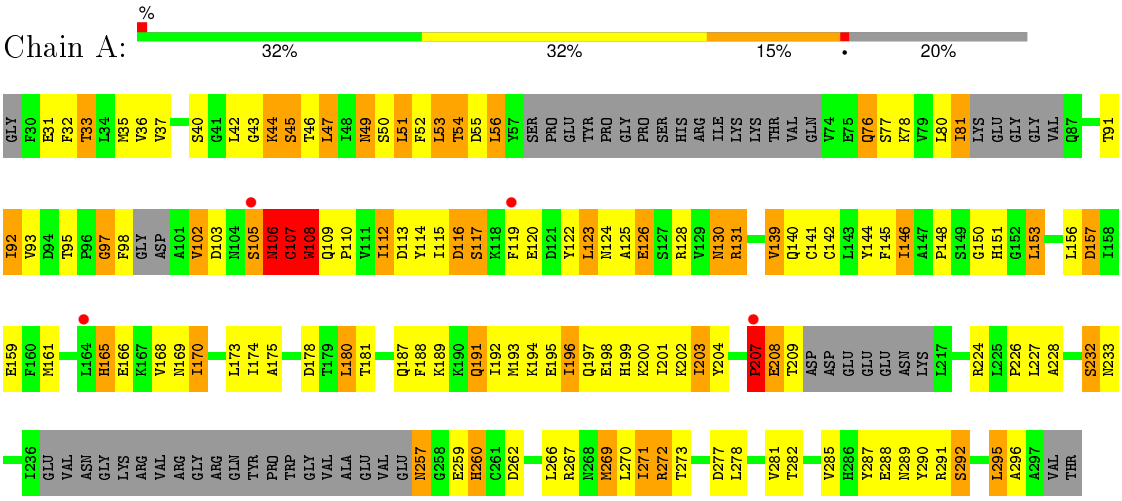
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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.

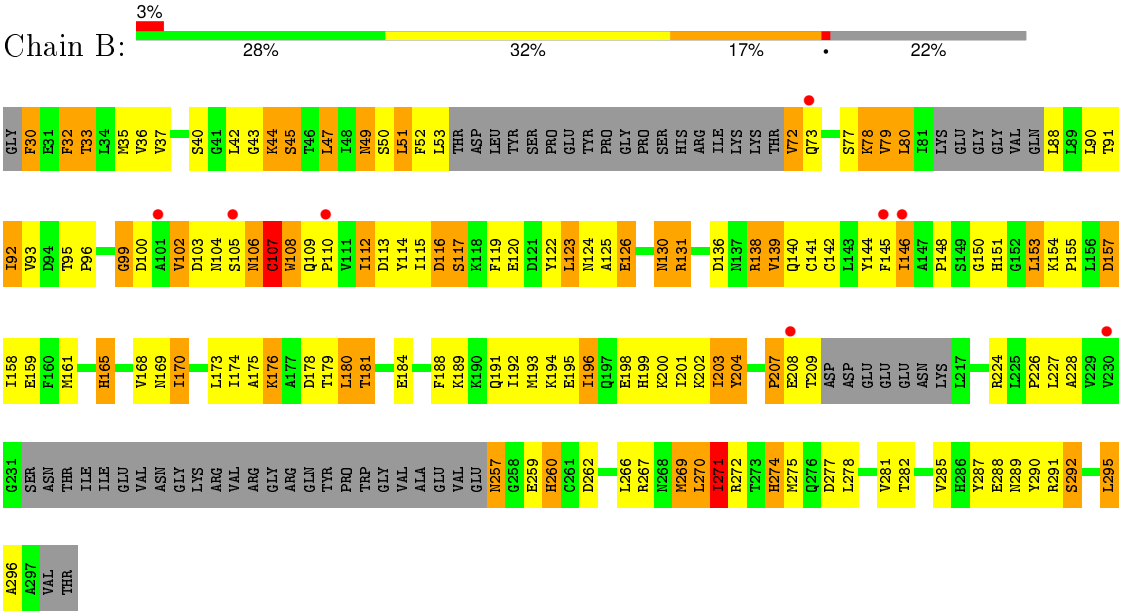
- Molecule 1: Septin-7

Chain A:



- Molecule 1: Septin-7

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	82.51Å 82.51Å 210.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.42 – 3.35 42.43 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.42-3.35) 98.7 (42.43-3.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.289 , 0.365 0.290 , 0.365	Depositor DCC
R_{free} test set	576 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	121.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 341.2	EDS
Estimated twinning fraction	0.430 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 11556 reflections (0.017%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3039	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: GDP

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	0.41	1/1533 (0.1%)	0.72	3/2094 (0.1%)
1	B	0.42	0/1496	0.70	3/2046 (0.1%)
All	All	0.42	1/3029 (0.0%)	0.71	6/4140 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	CYS	CB-SG	5.30	1.91	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	TRP	N-CA-C	-6.74	92.81	111.00
1	A	107	CYS	CB-CA-C	-6.59	97.22	110.40
1	B	150	GLY	N-CA-C	6.23	128.67	113.10
1	B	105	SER	N-CA-C	-5.84	95.23	111.00
1	A	150	GLY	N-CA-C	5.84	127.70	113.10
1	B	99	GLY	N-CA-C	-5.53	99.27	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ASN	Mainchain
1	A	107	CYS	Mainchain
1	A	207	PRO	Mainchain
1	A	232	SER	Peptide
1	A	55	ASP	Peptide
1	B	103	ASP	Peptide
1	B	107	CYS	Mainchain
1	B	207	PRO	Mainchain

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	1512	0	1291	122	3
1	B	1471	0	1274	134	3
2	A	28	0	12	9	0
2	B	28	0	12	11	0
All	All	3039	0	2589	255	3

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 46.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASP:OD2	2:B:501:GDP:N2	1.88	1.06
1:A:49:ASN:ND2	1:A:54:THR:O	1.95	1.00
1:A:106:ASN:O	1:A:107:CYS:O	1.80	0.98
1:B:153:LEU:HD22	1:B:158:ILE:HG13	1.49	0.93
1:B:106:ASN:O	1:B:107:CYS:O	1.89	0.90
1:A:49:ASN:HD21	1:A:56:LEU:H	1.20	0.88
1:B:271:ILE:HB	1:B:275:MET:CB	2.02	0.88
1:A:49:ASN:O	1:A:53:LEU:N	2.07	0.88
1:A:285:VAL:O	1:A:289:ASN:ND2	2.09	0.85
1:B:44:LYS:HB3	1:B:145:PHE:CZ	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HB3	1:A:145:PHE:CZ	2.13	0.83
1:B:285:VAL:O	1:B:289:ASN:ND2	2.11	0.83
1:A:107:CYS:SG	1:A:107:CYS:O	2.37	0.81
1:A:140:GLN:O	1:A:169:ASN:ND2	2.14	0.80
1:A:272:ARG:HE	1:A:273:THR:HA	1.48	0.78
1:B:140:GLN:O	1:B:169:ASN:ND2	2.16	0.77
1:A:43:GLY:HA2	2:A:500:GDP:PA	2.23	0.77
1:B:168:VAL:HG22	1:B:169:ASN:H	1.54	0.73
1:B:176:LYS:HG3	2:B:501:GDP:N1	2.02	0.73
1:B:49:ASN:O	1:B:53:LEU:N	2.21	0.72
1:A:168:VAL:HG22	1:A:169:ASN:H	1.55	0.72
1:A:43:GLY:N	2:A:500:GDP:O3A	2.23	0.71
1:B:196:ILE:HG22	1:B:201:ILE:HB	1.73	0.71
1:A:196:ILE:HG22	1:A:201:ILE:HB	1.73	0.70
1:A:156:LEU:HB2	1:B:102:VAL:HG21	1.72	0.70
1:B:195:GLU:O	1:B:199:HIS:ND1	2.21	0.69
1:B:176:LYS:HG3	2:B:501:GDP:C6	2.28	0.68
1:A:195:GLU:O	1:A:199:HIS:ND1	2.20	0.68
1:A:49:ASN:HD21	1:A:56:LEU:N	1.92	0.68
1:B:120:GLU:HB2	1:B:290:TYR:OH	1.94	0.67
1:A:120:GLU:HB2	1:A:290:TYR:OH	1.94	0.67
1:A:37:VAL:HG12	1:A:144:TYR:CD1	2.29	0.67
1:A:76:GLN:HA	1:A:92:ILE:O	1.95	0.66
1:A:112:ILE:HG22	1:A:113:ASP:N	2.12	0.65
1:B:112:ILE:HG22	1:B:113:ASP:N	2.11	0.65
1:B:267:ARG:O	1:B:270:LEU:HD23	1.97	0.65
1:B:176:LYS:HD2	2:B:501:GDP:C4	2.32	0.65
1:B:43:GLY:HA2	2:B:501:GDP:PA	2.37	0.64
1:A:44:LYS:HB3	1:A:145:PHE:CE1	2.32	0.64
1:B:181:THR:HG23	1:B:184:GLU:OE1	1.97	0.63
1:B:37:VAL:HG12	1:B:144:TYR:CD1	2.32	0.63
1:B:178:ASP:OD2	2:B:501:GDP:C2	2.51	0.63
1:A:108:TRP:N	1:A:110:PRO:HD2	2.13	0.63
1:B:106:ASN:C	1:B:107:CYS:O	2.32	0.63
1:B:44:LYS:HB3	1:B:145:PHE:CE1	2.33	0.63
1:A:105:SER:OG	1:A:106:ASN:N	2.30	0.62
1:A:119:PHE:HB3	1:A:290:TYR:CD2	2.34	0.62
1:B:119:PHE:HB3	1:B:290:TYR:CD2	2.35	0.62
1:A:108:TRP:H	1:A:110:PRO:HD2	1.64	0.62
1:A:288:GLU:OE1	1:A:292:SER:OG	2.15	0.62
1:B:271:ILE:O	1:B:274:HIS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD12	1:B:271:ILE:H	1.65	0.61
1:B:176:LYS:HD2	2:B:501:GDP:C5	2.36	0.61
1:B:178:ASP:CG	2:B:501:GDP:HN21	2.01	0.61
1:A:35:MET:HA	1:A:93:VAL:HB	1.82	0.61
2:A:500:GDP:O2'	1:B:184:GLU:OE2	2.17	0.61
1:A:119:PHE:HB3	1:A:290:TYR:CE2	2.36	0.61
1:B:77:SER:HB3	1:B:92:ILE:HG22	1.83	0.61
1:B:288:GLU:OE1	1:B:292:SER:OG	2.19	0.61
1:A:130:ASN:OD1	1:A:130:ASN:N	2.34	0.61
1:B:73:GLN:O	1:B:96:PRO:HD2	2.01	0.60
1:B:119:PHE:HB3	1:B:290:TYR:CE2	2.36	0.60
1:B:130:ASN:N	1:B:130:ASN:OD1	2.35	0.59
1:A:51:LEU:HB2	1:A:52:PHE:CD2	2.37	0.59
1:A:174:ILE:N	1:A:227:LEU:O	2.23	0.59
1:A:148:PRO:HB3	1:A:175:ALA:O	2.03	0.59
1:A:51:LEU:HD13	1:A:52:PHE:CZ	2.38	0.59
1:B:291:ARG:O	1:B:295:LEU:HD23	2.02	0.58
1:B:153:LEU:CD1	1:B:192:ILE:HG23	2.33	0.58
1:B:115:ILE:HD13	1:B:139:VAL:HG21	1.85	0.58
1:A:153:LEU:CD1	1:A:192:ILE:HG23	2.33	0.58
1:B:259:GLU:OE1	1:B:260:HIS:ND1	2.36	0.58
1:B:51:LEU:HD13	1:B:52:PHE:CZ	2.39	0.58
1:A:42:LEU:HD13	1:A:145:PHE:CB	2.34	0.58
1:A:291:ARG:O	1:A:295:LEU:HD23	2.03	0.58
1:B:257:ASN:N	1:B:257:ASN:HD22	2.00	0.57
1:B:178:ASP:CG	2:B:501:GDP:HN1	2.08	0.57
1:A:259:GLU:OE1	1:A:260:HIS:ND1	2.37	0.57
1:B:51:LEU:HB2	1:B:52:PHE:CD2	2.39	0.57
1:B:153:LEU:CD2	1:B:158:ILE:HG13	2.30	0.57
1:A:80:LEU:C	1:A:81:ILE:HG13	2.25	0.57
1:B:174:ILE:N	1:B:227:LEU:O	2.23	0.56
1:A:42:LEU:HD13	1:A:145:PHE:HB2	1.88	0.56
1:B:119:PHE:CD2	1:B:138:ARG:HG2	2.41	0.56
1:A:153:LEU:HD11	1:A:192:ILE:HG23	1.88	0.55
1:B:153:LEU:HD11	1:B:192:ILE:HG23	1.87	0.55
1:A:78:LYS:HD3	1:A:78:LYS:N	2.22	0.55
1:B:42:LEU:HD13	1:B:145:PHE:CB	2.36	0.55
1:A:45:SER:HB3	2:A:500:GDP:O1B	2.07	0.55
1:B:148:PRO:HB3	1:B:175:ALA:O	2.07	0.55
1:B:42:LEU:HD13	1:B:145:PHE:HB2	1.89	0.55
1:A:108:TRP:HD1	1:A:109:GLN:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:O	1:A:126:GLU:N	2.40	0.54
1:A:43:GLY:HA2	2:A:500:GDP:O5'	2.07	0.54
1:B:107:CYS:O	1:B:108:TRP:CG	2.60	0.54
1:B:123:LEU:O	1:B:126:GLU:N	2.40	0.54
1:B:277:ASP:O	1:B:281:VAL:HG23	2.07	0.54
1:A:123:LEU:HD23	1:A:124:ASN:N	2.22	0.54
1:A:270:LEU:O	1:A:271:ILE:C	2.47	0.54
1:A:140:GLN:HA	1:A:282:THR:OG1	2.08	0.53
1:A:187:GLN:O	1:A:191:GLN:HB2	2.07	0.53
1:B:140:GLN:HA	1:B:282:THR:OG1	2.07	0.53
1:B:153:LEU:HD23	1:B:157:ASP:HB2	1.91	0.53
1:A:51:LEU:HB2	1:A:52:PHE:CE2	2.44	0.53
1:B:32:PHE:CD1	1:B:271:ILE:HG21	2.44	0.53
1:A:196:ILE:O	1:A:200:LYS:N	2.42	0.53
1:A:33:THR:OG1	1:A:139:VAL:HA	2.09	0.53
1:B:287:TYR:O	1:B:290:TYR:HB3	2.09	0.53
1:B:35:MET:HA	1:B:93:VAL:HB	1.90	0.53
1:B:123:LEU:HD23	1:B:124:ASN:N	2.24	0.53
1:B:196:ILE:O	1:B:200:LYS:N	2.43	0.52
1:B:108:TRP:N	1:B:110:PRO:HD2	2.25	0.52
1:A:277:ASP:O	1:A:281:VAL:HG23	2.09	0.52
1:A:203:ILE:HG12	1:A:204:TYR:N	2.24	0.52
1:A:191:GLN:O	1:A:195:GLU:HG2	2.10	0.52
1:A:116:ASP:OD1	1:A:116:ASP:N	2.42	0.52
1:A:115:ILE:HD13	1:A:139:VAL:HG21	1.91	0.52
1:B:165:HIS:ND1	1:B:201:ILE:HG23	2.25	0.51
1:B:136:ASP:OD1	1:B:138:ARG:NE	2.43	0.51
1:A:287:TYR:O	1:A:290:TYR:HB3	2.10	0.51
1:B:115:ILE:CD1	1:B:139:VAL:HG21	2.40	0.51
1:B:191:GLN:O	1:B:195:GLU:HG2	2.10	0.51
1:B:45:SER:HB3	2:B:501:GDP:O3B	2.11	0.51
1:B:51:LEU:HB2	1:B:52:PHE:CE2	2.45	0.51
1:B:203:ILE:HG12	1:B:204:TYR:N	2.24	0.51
1:A:97:GLY:O	1:A:98:PHE:O	2.29	0.51
1:A:266:LEU:HG	1:A:267:ARG:N	2.26	0.50
1:A:266:LEU:O	1:A:269:MET:N	2.43	0.50
1:B:37:VAL:HG22	1:B:95:THR:HG21	1.93	0.50
1:B:266:LEU:HG	1:B:267:ARG:N	2.26	0.50
1:B:116:ASP:OD1	1:B:116:ASP:N	2.43	0.50
1:B:189:LYS:HA	1:B:192:ILE:HD12	1.93	0.50
1:A:146:ILE:HG12	1:A:173:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:MET:HA	1:B:196:ILE:HG13	1.93	0.49
1:A:49:ASN:N	1:A:49:ASN:OD1	2.45	0.49
1:A:194:LYS:O	1:A:198:GLU:HB3	2.13	0.49
1:B:270:LEU:O	1:B:271:ILE:C	2.49	0.49
1:B:266:LEU:O	1:B:269:MET:N	2.46	0.49
1:B:271:ILE:HG12	1:B:272:ARG:N	2.27	0.49
1:B:77:SER:HB3	1:B:92:ILE:CG2	2.42	0.49
1:B:33:THR:OG1	1:B:139:VAL:HA	2.12	0.49
1:B:189:LYS:NZ	1:B:224:ARG:O	2.45	0.49
1:A:165:HIS:HA	1:A:170:ILE:HD11	1.94	0.49
1:A:257:ASN:HD22	1:A:257:ASN:N	2.10	0.49
1:B:271:ILE:HG12	1:B:272:ARG:H	1.77	0.49
1:B:49:ASN:OD1	1:B:49:ASN:N	2.45	0.49
1:A:49:ASN:ND2	1:A:56:LEU:H	1.99	0.48
1:B:168:VAL:HG22	1:B:169:ASN:N	2.27	0.48
1:B:194:LYS:O	1:B:198:GLU:HB3	2.12	0.48
1:A:193:MET:HA	1:A:196:ILE:HG13	1.93	0.48
1:B:165:HIS:HA	1:B:170:ILE:HD11	1.96	0.48
1:A:165:HIS:CD2	1:A:166:GLU:HG2	2.48	0.48
1:A:189:LYS:HA	1:A:192:ILE:HD12	1.94	0.48
1:A:165:HIS:ND1	1:A:201:ILE:HG23	2.29	0.48
1:B:267:ARG:HG2	1:B:270:LEU:HD23	1.94	0.48
1:A:46:THR:HG23	2:A:500:GDP:O1A	2.13	0.48
1:A:153:LEU:HD23	1:A:157:ASP:HB2	1.94	0.48
1:A:193:MET:SD	1:A:226:PRO:HD3	2.54	0.48
1:A:37:VAL:HG22	1:A:95:THR:HG21	1.94	0.48
1:A:115:ILE:CD1	1:A:139:VAL:HG21	2.43	0.48
1:B:146:ILE:HG12	1:B:173:LEU:O	2.13	0.48
1:B:192:ILE:O	1:B:195:GLU:N	2.47	0.48
1:A:43:GLY:CA	2:A:500:GDP:O3A	2.62	0.48
1:B:193:MET:SD	1:B:226:PRO:HD3	2.54	0.47
1:A:106:ASN:O	1:A:107:CYS:C	2.47	0.47
1:A:271:ILE:O	1:A:272:ARG:HD2	2.15	0.47
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.58	0.47
1:A:192:ILE:O	1:A:195:GLU:N	2.48	0.47
1:B:122:TYR:O	1:B:125:ALA:HB3	2.15	0.46
1:A:140:GLN:OE1	1:A:140:GLN:N	2.47	0.46
1:B:102:VAL:HG23	1:B:102:VAL:O	2.16	0.46
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.58	0.46
1:A:77:SER:H	1:A:92:ILE:HG22	1.81	0.46
1:A:295:LEU:O	1:A:296:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD12	1:B:271:ILE:HG23	1.97	0.46
1:B:109:GLN:N	1:B:110:PRO:CD	2.78	0.46
1:A:42:LEU:HD13	1:A:145:PHE:HB3	1.97	0.46
1:A:108:TRP:HD1	1:A:109:GLN:N	2.13	0.46
1:B:196:ILE:O	1:B:199:HIS:N	2.49	0.45
1:B:201:ILE:HG22	1:B:202:LYS:N	2.31	0.45
1:A:201:ILE:HG22	1:A:202:LYS:N	2.31	0.45
1:B:108:TRP:O	1:B:112:ILE:HD13	2.16	0.45
1:B:30:PHE:HE2	1:B:272:ARG:O	1.98	0.45
1:A:189:LYS:NZ	1:A:224:ARG:O	2.45	0.45
1:B:295:LEU:O	1:B:296:ALA:C	2.54	0.45
1:B:192:ILE:O	1:B:195:GLU:HB2	2.16	0.45
1:B:95:THR:O	1:B:95:THR:OG1	2.34	0.45
1:A:49:ASN:CG	1:A:54:THR:O	2.55	0.45
1:A:168:VAL:HG22	1:A:169:ASN:N	2.28	0.45
1:B:114:TYR:O	1:B:117:SER:HB3	2.16	0.45
1:A:141:CYS:HB2	1:A:278:LEU:HD13	1.98	0.45
1:B:99:GLY:O	1:B:100:ASP:C	2.54	0.45
1:B:140:GLN:OE1	1:B:140:GLN:N	2.49	0.45
1:A:47:LEU:O	1:A:50:SER:HB3	2.17	0.45
1:B:43:GLY:N	2:B:501:GDP:O3A	2.43	0.44
2:A:500:GDP:HN22	1:B:179:THR:HG23	1.82	0.44
1:B:36:VAL:HG22	1:B:93:VAL:O	2.16	0.44
1:B:80:LEU:HA	1:B:88:LEU:O	2.17	0.44
1:A:122:TYR:O	1:A:125:ALA:HB3	2.17	0.44
1:B:141:CYS:HB2	1:B:278:LEU:HD13	1.99	0.44
1:A:37:VAL:CG1	1:A:144:TYR:CD1	3.00	0.44
1:A:44:LYS:O	1:A:47:LEU:N	2.51	0.44
1:B:204:TYR:CE2	1:B:278:LEU:HD21	2.53	0.44
1:B:47:LEU:O	1:B:50:SER:HB3	2.18	0.44
1:B:52:PHE:CD2	1:B:52:PHE:N	2.85	0.44
1:A:196:ILE:O	1:A:199:HIS:N	2.51	0.43
1:A:178:ASP:OD1	2:A:500:GDP:N1	2.49	0.43
1:A:165:HIS:HB2	1:A:202:LYS:O	2.17	0.43
1:B:77:SER:OG	1:B:78:LYS:N	2.52	0.43
1:B:79:VAL:HG12	1:B:90:LEU:HB2	2.01	0.43
1:B:108:TRP:HZ3	1:B:159:GLU:CB	2.32	0.43
1:A:287:TYR:CD1	1:A:287:TYR:C	2.90	0.43
1:A:114:TYR:O	1:A:117:SER:HB3	2.18	0.43
1:B:47:LEU:HA	1:B:50:SER:CB	2.49	0.43
1:B:119:PHE:HD2	1:B:138:ARG:HG2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:O	1:A:195:GLU:HB2	2.18	0.43
1:B:42:LEU:HD13	1:B:145:PHE:HB3	2.01	0.42
1:A:50:SER:OG	1:A:232:SER:O	2.33	0.42
1:A:108:TRP:HZ3	1:A:159:GLU:CB	2.32	0.42
1:A:36:VAL:HG22	1:A:93:VAL:O	2.18	0.42
1:A:52:PHE:N	1:A:52:PHE:CD2	2.84	0.42
1:B:228:ALA:O	1:B:262:ASP:HB2	2.19	0.42
1:B:44:LYS:O	1:B:47:LEU:N	2.52	0.42
1:B:271:ILE:CG1	1:B:272:ARG:N	2.82	0.42
1:A:144:TYR:OH	1:A:157:ASP:HA	2.19	0.42
1:B:72:VAL:HG12	1:B:73:GLN:H	1.84	0.42
1:A:49:ASN:ND2	1:A:56:LEU:N	2.63	0.42
1:B:165:HIS:HB2	1:B:202:LYS:O	2.19	0.42
1:B:189:LYS:HB3	1:B:226:PRO:HD2	2.00	0.42
1:A:47:LEU:HA	1:A:50:SER:CB	2.49	0.42
1:B:35:MET:CE	1:B:93:VAL:HG11	2.49	0.42
1:A:189:LYS:HB3	1:A:226:PRO:HD2	2.01	0.42
1:B:287:TYR:CD1	1:B:287:TYR:C	2.92	0.42
1:B:154:LYS:HA	1:B:155:PRO:HD3	1.87	0.42
1:A:102:VAL:HG12	1:A:103:ASP:N	2.34	0.42
1:B:193:MET:CG	1:B:226:PRO:HD3	2.49	0.42
1:A:193:MET:CG	1:A:226:PRO:HD3	2.50	0.42
1:A:35:MET:CE	1:A:93:VAL:HG11	2.50	0.42
1:B:153:LEU:HD22	1:B:158:ILE:CG1	2.37	0.41
1:A:95:THR:O	1:A:95:THR:OG1	2.35	0.41
1:A:122:TYR:CE2	1:A:287:TYR:CE2	3.08	0.41
1:B:144:TYR:OH	1:B:157:ASP:HA	2.20	0.41
1:A:109:GLN:HA	1:A:112:ILE:HB	2.02	0.41
1:A:228:ALA:O	1:A:262:ASP:HB2	2.20	0.41
1:B:145:PHE:N	1:B:145:PHE:CD2	2.88	0.41
1:B:32:PHE:HD1	1:B:271:ILE:HG21	1.85	0.40
1:A:44:LYS:H	1:A:44:LYS:HG2	1.67	0.40
1:A:47:LEU:HA	1:A:50:SER:HB3	2.02	0.40
1:B:138:ARG:HB2	1:B:138:ARG:HE	1.62	0.40
1:A:35:MET:O	1:A:142:CYS:HA	2.21	0.40
1:B:35:MET:O	1:B:142:CYS:HA	2.22	0.40
1:B:37:VAL:HG12	1:B:37:VAL:O	2.22	0.40
1:A:178:ASP:N	1:A:178:ASP:OD1	2.54	0.40
1:A:153:LEU:HD12	1:A:192:ILE:HG23	2.04	0.40
1:A:207:PRO:O	1:A:208:GLU:O	2.39	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:NH1	1:B:126:GLU:OE1[1_445]	2.16	0.04
1:A:126:GLU:OE1	1:B:131:ARG:NH1[1_445]	2.18	0.02
1:A:81:ILE:N	1:B:80:LEU:O[6_555]	2.19	0.01

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	206/271 (76%)	160 (78%)	36 (18%)	10 (5%)	3	22
1	B	202/271 (74%)	158 (78%)	37 (18%)	7 (4%)	4	32
All	All	408/542 (75%)	318 (78%)	73 (18%)	17 (4%)	3	27

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	GLU
1	B	107	CYS
1	B	207	PRO
1	B	208	GLU
1	A	107	CYS
1	A	207	PRO
1	A	97	GLY
1	A	105	SER
1	A	108	TRP
1	A	102	VAL
1	A	106	ASN
1	B	106	ASN
1	B	271	ILE
1	B	102	VAL
1	A	112	ILE
1	A	271	ILE

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Mol	Chain	Res	Type
1	B	112	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	132/246 (54%)	85 (64%)	47 (36%)	0 1
1	B	127/246 (52%)	79 (62%)	48 (38%)	0 0
All	All	259/492 (53%)	164 (63%)	95 (37%)	0 1

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	32	PHE
1	A	33	THR
1	A	40	SER
1	A	44	LYS
1	A	45	SER
1	A	47	LEU
1	A	49	ASN
1	A	51	LEU
1	A	53	LEU
1	A	54	THR
1	A	56	LEU
1	A	76	GLN
1	A	81	ILE
1	A	91	THR
1	A	92	ILE
1	A	108	TRP
1	A	116	ASP
1	A	117	SER
1	A	123	LEU
1	A	126	GLU
1	A	128	ARG

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Mol	Chain	Res	Type
1	A	130	ASN
1	A	131	ARG
1	A	139	VAL
1	A	146	ILE
1	A	151	HIS
1	A	153	LEU
1	A	157	ASP
1	A	161	MET
1	A	165	HIS
1	A	170	ILE
1	A	180	LEU
1	A	181	THR
1	A	188	PHE
1	A	191	GLN
1	A	196	ILE
1	A	197	GLN
1	A	203	ILE
1	A	209	THR
1	A	233	ASN
1	A	257	ASN
1	A	260	HIS
1	A	269	MET
1	A	272	ARG
1	A	292	SER
1	A	295	LEU
1	B	30	PHE
1	B	32	PHE
1	B	33	THR
1	B	40	SER
1	B	44	LYS
1	B	45	SER
1	B	47	LEU
1	B	49	ASN
1	B	51	LEU
1	B	72	VAL
1	B	78	LYS
1	B	79	VAL
1	B	80	LEU
1	B	91	THR
1	B	92	ILE
1	B	104	ASN
1	B	108	TRP

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Mol	Chain	Res	Type
1	B	116	ASP
1	B	117	SER
1	B	123	LEU
1	B	126	GLU
1	B	130	ASN
1	B	131	ARG
1	B	138	ARG
1	B	139	VAL
1	B	146	ILE
1	B	151	HIS
1	B	153	LEU
1	B	157	ASP
1	B	161	MET
1	B	165	HIS
1	B	170	ILE
1	B	176	LYS
1	B	180	LEU
1	B	181	THR
1	B	188	PHE
1	B	196	ILE
1	B	203	ILE
1	B	204	TYR
1	B	209	THR
1	B	257	ASN
1	B	260	HIS
1	B	269	MET
1	B	270	LEU
1	B	271	ILE
1	B	274	HIS
1	B	292	SER
1	B	295	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	A	500	-	23,30,30	1.13	2 (8%)	30,47,47	1.92	7 (23%)
2	GDP	B	501	-	23,30,30	1.10	2 (8%)	30,47,47	2.04	8 (26%)

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
2	GDP	A	500	-	-	0/12/32/32	0/3/3/3
2	GDP	B	501	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GDP	C5-C4	2.81	1.46	1.40
2	A	500	GDP	C5-C4	2.94	1.47	1.40
2	B	501	GDP	C6-C5	3.37	1.48	1.41
2	A	500	GDP	C6-C5	3.57	1.48	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	GDP	C5-C6-N1	-4.53	117.39	123.59
2	A	500	GDP	C5-C6-N1	-4.22	117.81	123.59
2	B	501	GDP	C2'-C1'-N9	-3.99	108.19	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	GDP	C2'-C1'-N9	-3.68	108.67	114.29
2	B	501	GDP	C6-C5-C4	-3.64	116.55	120.90
2	A	500	GDP	C6-C5-C4	-3.41	116.82	120.90
2	B	501	GDP	N3-C2-N1	-3.15	122.65	127.44
2	A	500	GDP	N3-C2-N1	-3.10	122.72	127.44
2	B	501	GDP	C4-C5-N7	-3.08	106.65	109.48
2	A	500	GDP	PA-O3A-PB	-2.89	122.97	132.67
2	B	501	GDP	PA-O3A-PB	-2.83	123.19	132.67
2	A	500	GDP	C4-C5-N7	-2.81	106.89	109.48
2	B	501	GDP	C1'-N9-C4	-2.52	123.14	126.94
2	A	500	GDP	C6-N1-C2	4.89	122.73	115.94
2	B	501	GDP	C6-N1-C2	4.98	122.85	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	GDP	9	0
2	B	501	GDP	11	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	216/271 (79%)	-0.21	4 (1%) 70 70	73, 141, 231, 316	0
1	B	210/271 (77%)	-0.17	8 (3%) 44 44	60, 137, 232, 392	0
All	All	426/542 (78%)	-0.19	12 (2%) 56 57	60, 138, 232, 392	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	PRO	4.6
1	B	105	SER	3.9
1	B	145	PHE	3.1
1	A	105	SER	2.6
1	B	230	VAL	2.5
1	A	164	LEU	2.5
1	A	119	PHE	2.4
1	B	73	GLN	2.4
1	B	208	GLU	2.3
1	B	146	ILE	2.2
1	B	110	PRO	2.0
1	B	101	ALA	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. 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
2	GDP	A	500	28/28	0.95	0.20	-0.09	49,132,145,155	0
2	GDP	B	501	28/28	0.94	0.18	-0.51	59,138,150,153	0

6.5 Other polymers

There are no such residues in this entry.