Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2016 – 12:01 PM EDT

PDB ID	:	5APL
Title	:	Structure of the adenylation domain THR1 involved in the biosynthesis of 4-chlorothreonine in streptomyces sp. Oh-5093, apo structure
Authors	:	Savino, C.; Scaglione, A.; Montemiglio, L.C.; Parisi, G.; Grgurina, I.; Fullone, M.R.; Vallone, B.
Deposited on	:	2015-09-16
Resolution	:	2.46 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:

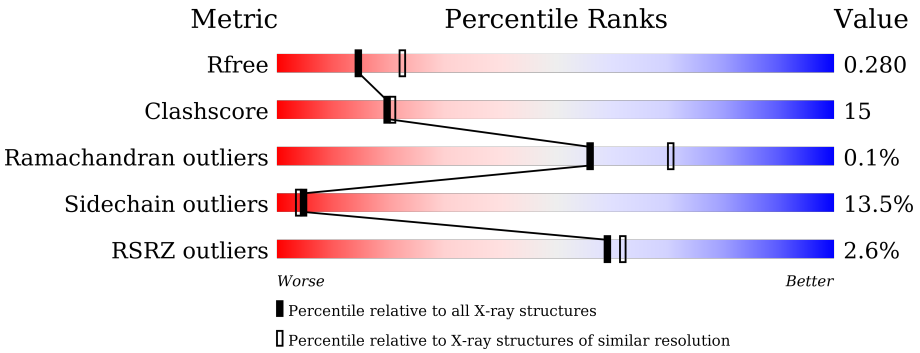
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.46 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	529	2% 62% 25% 6% 8%
1	B	529	3% 63% 25% 5% 6%

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	ACT	A	1530	-	-	-	X
2	ACT	B	1531	-	-	X	X

2 Entry composition

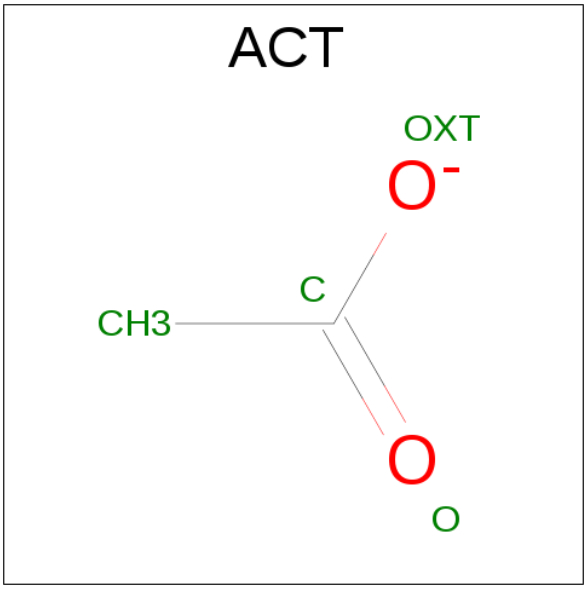
There are 3 unique types of molecules in this entry. The entry contains 7691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADENYLATION DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	1	0
			3763	2378	679	697	9			
1	B	496	Total	C	N	O	S	0	3	0
			3836	2423	690	714	9			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

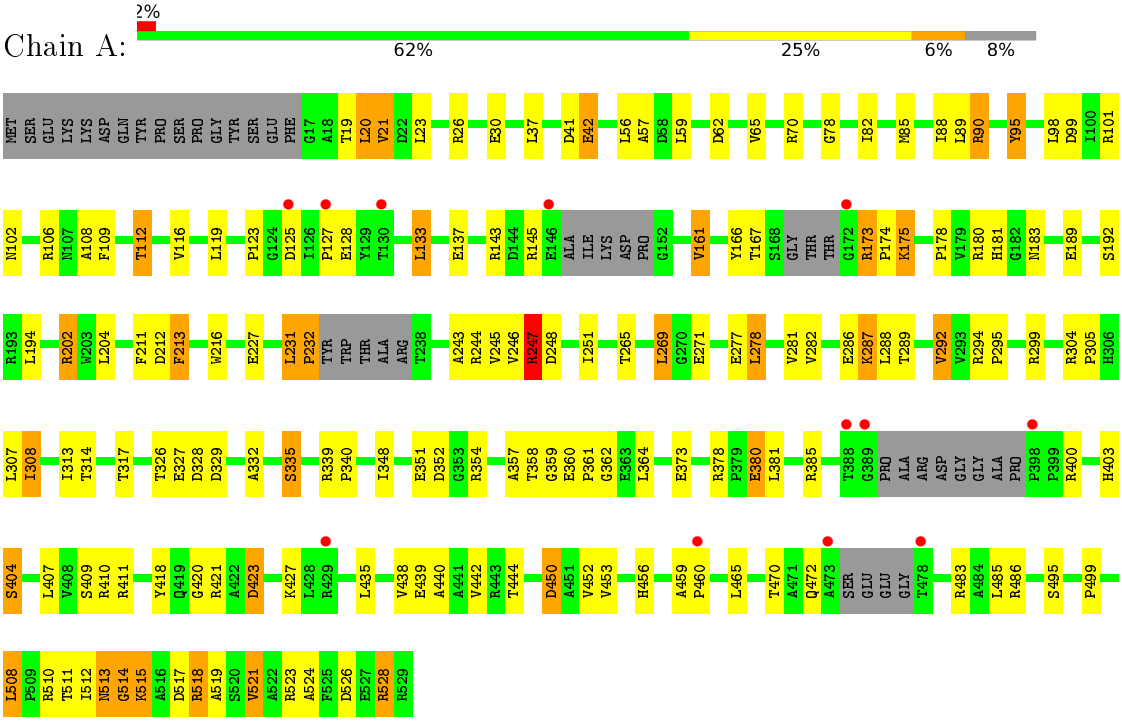
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	41	Total O 41 41	0	0

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.

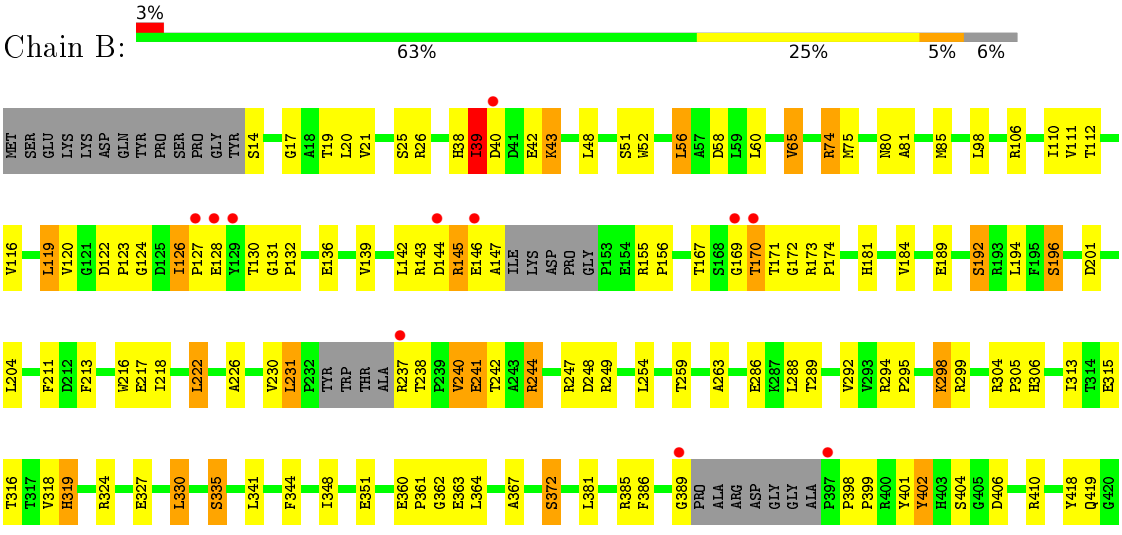
- Molecule 1: ADENYLATION DOMAIN

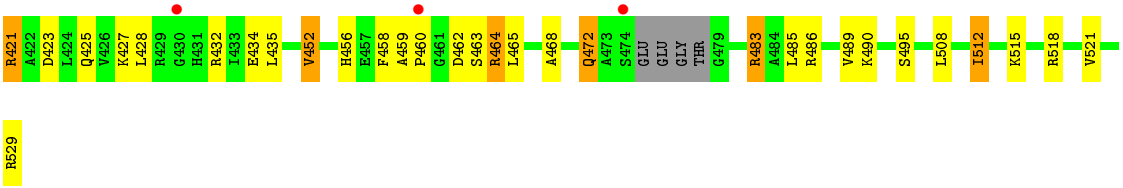
Chain A:



- Molecule 1: ADENYLATION DOMAIN

Chain B:




R421
A422
D423
L424
Q425
V426
K427
L428
R429
G430
H431
R432
I433
E434
L435
V452
H456
E457
F458
A459
P460
G461
D462
S463
R464
L465
A468
Q472
A473
S474
GLU
GLU
GLY
THR
G479
R483
A484
L485
R486
V489
K490
S495
L508
I512
K515
R518
V521
R529

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.63Å 52.81Å 108.86Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	46.95 – 2.46 46.95 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.95-2.46) 99.7 (46.95-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.249 , 0.316 0.218 , 0.280	Depositor DCC
R_{free} test set	1788 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7691	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.22% 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, 0.333 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: ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.47	6/3853 (0.2%)	0.92	6/5247 (0.1%)
1	B	1.50	14/3935 (0.4%)	0.94	9/5359 (0.2%)
All	All	1.49	20/7788 (0.3%)	0.93	15/10606 (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	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241[A]	GLU	N-CA	11.62	1.69	1.46
1	B	241[B]	GLU	N-CA	11.62	1.69	1.46
1	B	58[A]	ASP	N-CA	9.10	1.64	1.46
1	B	58[B]	ASP	N-CA	9.10	1.64	1.46
1	A	515[A]	LYS	CA-C	7.69	1.73	1.52
1	A	515[B]	LYS	CA-C	7.69	1.73	1.52
1	B	515[A]	LYS	CA-C	7.24	1.71	1.52
1	B	515[B]	LYS	CA-C	7.24	1.71	1.52
1	A	216	TRP	NE1-CE2	-5.83	1.29	1.37
1	A	232	PRO	N-CD	5.75	1.55	1.47
1	B	402	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	52	TRP	NE1-CE2	-5.43	1.30	1.37
1	B	363	GLU	CD-OE1	-5.37	1.19	1.25
1	A	95	TYR	CE1-CZ	-5.32	1.31	1.38
1	B	217	GLU	CD-OE2	-5.19	1.20	1.25
1	B	319	HIS	CG-ND1	-5.17	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLU	CD-OE2	-5.13	1.20	1.25
1	B	418	TYR	CE1-CZ	-5.12	1.31	1.38
1	B	132	PRO	N-CD	5.07	1.54	1.47
1	B	216	TRP	NE1-CE2	-5.01	1.31	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	515[A]	LYS	CA-C-N	-8.47	98.56	117.20
1	A	515[B]	LYS	CA-C-N	-8.47	98.56	117.20
1	B	231	LEU	C-N-CD	6.34	141.71	128.40
1	B	126	ILE	C-N-CD	6.08	141.16	128.40
1	B	241[A]	GLU	CA-C-O	6.01	132.72	120.10
1	B	241[B]	GLU	CA-C-O	6.01	132.72	120.10
1	B	240	VAL	C-N-CA	-5.96	106.80	121.70
1	A	515[A]	LYS	CA-C-O	5.75	132.17	120.10
1	A	515[B]	LYS	CA-C-O	5.75	132.17	120.10
1	B	131	GLY	C-N-CD	5.41	139.75	128.40
1	A	231	LEU	C-N-CD	5.36	139.65	128.40
1	B	241[A]	GLU	CA-C-N	-5.30	105.54	117.20
1	B	241[B]	GLU	CA-C-N	-5.30	105.54	117.20
1	A	247	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	39	ILE	CB-CA-C	-5.10	101.39	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	514	GLY	Peptide
1	A	515[A]	LYS	Mainchain
1	A	515[B]	LYS	Mainchain

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	3763	0	3721	103	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3836	0	3788	124	1
2	A	4	0	3	0	0
2	B	8	0	6	3	0
3	A	39	0	0	3	0
3	B	41	0	0	1	0
All	All	7691	0	7518	226	1

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 15.

All (226) 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:288:LEU:O	1:B:335:SER:OG	1.63	1.15
1:B:155:ARG:NH2	3:B:2010:HOH:O	1.88	1.06
1:B:485:LEU:O	1:B:489:VAL:HG23	1.56	1.06
1:A:102:ASN:OD1	1:A:106:ARG:NH1	1.91	1.03
1:B:74:ARG:HH12	1:B:124:GLY:HA3	1.34	0.90
1:B:240:VAL:C	1:B:241[A]:GLU:CA	2.42	0.88
1:B:240:VAL:C	1:B:241[B]:GLU:CA	2.42	0.88
1:B:259:THR:OG1	1:B:286:GLU:OE2	1.89	0.88
1:A:517:ASP:O	1:A:521:VAL:HG23	1.76	0.84
1:A:380:GLU:OE1	1:A:381:LEU:N	2.11	0.83
1:A:127:PRO:C	1:A:128:GLU:HG3	1.99	0.83
1:A:326:THR:HG22	1:A:327:GLU:H	1.42	0.82
1:B:289:THR:O	1:B:292:VAL:HG12	1.81	0.81
1:B:123:PRO:HD2	1:B:124:GLY:H	1.47	0.80
1:A:173:ARG:HG2	1:A:173:ARG:NH1	1.98	0.78
1:B:145:ARG:NH2	1:B:147:ALA:HA	1.99	0.78
1:A:173:ARG:HG2	1:A:173:ARG:HH11	1.48	0.78
1:A:364:LEU:O	1:A:404:SER:OG	2.02	0.77
1:A:326:THR:HG22	1:A:327:GLU:N	2.00	0.76
1:A:357:ALA:N	1:A:360:GLU:OE1	2.19	0.76
1:A:304:ARG:NH1	3:A:2026:HOH:O	2.18	0.74
1:B:432:ARG:HG3	1:B:432:ARG:HH11	1.51	0.74
1:A:174:PRO:O	1:A:378:ARG:NH2	2.20	0.73
1:A:517:ASP:O	1:A:521:VAL:CG2	2.36	0.73
1:A:108:ALA:O	1:A:112:THR:HG22	1.89	0.73
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.52	0.72
1:A:339:ARG:HD3	1:A:340:PRO:HD2	1.71	0.71
1:B:145:ARG:HH22	1:B:147:ALA:HA	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HH22	1:A:512:ILE:HD12	1.56	0.70
1:A:442:VAL:HG13	1:A:485:LEU:HD11	1.73	0.70
1:A:439:GLU:OE2	1:A:518:ARG:NH2	2.24	0.70
1:B:111:VAL:HG23	1:B:116:VAL:CG2	2.22	0.69
1:B:427:LYS:HD2	1:B:432:ARG:NH2	2.09	0.68
1:A:456:HIS:CE1	1:A:526:ASP:OD1	2.47	0.68
1:A:440:ALA:O	1:A:444:THR:HG23	1.94	0.67
1:A:435:LEU:HD22	1:A:453:VAL:HG23	1.76	0.66
1:A:247:ARG:HG3	1:A:248:ASP:N	2.11	0.66
1:A:328:ASP:OD1	1:A:329:ASP:N	2.29	0.65
1:B:483:ARG:CG	1:B:483:ARG:HH11	2.09	0.65
1:A:352:ASP:OD1	1:A:354:ARG:NH1	2.30	0.65
1:A:202:ARG:HG3	1:A:227:GLU:HB3	1.79	0.65
1:B:294:ARG:NH1	1:B:330:LEU:O	2.29	0.65
1:B:123:PRO:CD	1:B:124:GLY:H	2.09	0.65
1:B:145:ARG:HH11	1:B:145:ARG:CG	2.10	0.65
1:A:470:THR:HG23	1:A:508:LEU:HD13	1.79	0.65
1:A:59:LEU:O	1:A:62:ASP:HB2	1.97	0.65
1:B:111:VAL:HG23	1:B:116:VAL:HG22	1.80	0.64
1:A:204:LEU:HD11	1:A:231:LEU:HG	1.80	0.64
1:A:518:ARG:HH11	1:A:518:ARG:HG3	1.63	0.63
1:B:247:ARG:NH1	1:B:248:ASP:OD1	2.29	0.63
1:A:410:ARG:HG2	1:A:411:ARG:O	2.00	0.62
1:A:42:GLU:OE2	1:A:143:ARG:NH2	2.28	0.62
1:B:136:GLU:O	1:B:139:VAL:HG22	1.98	0.61
1:B:204:LEU:HD11	1:B:231:LEU:HG	1.82	0.61
1:B:289:THR:O	1:B:292:VAL:CG1	2.49	0.61
1:B:119:LEU:HD23	1:B:120:VAL:N	2.16	0.60
1:B:39:ILE:O	1:B:42:GLU:HB2	2.01	0.60
1:A:108:ALA:O	1:A:112:THR:CG2	2.49	0.60
1:A:278:LEU:HD12	1:A:305:PRO:HG3	1.84	0.59
1:B:240:VAL:O	1:B:241[A]:GLU:CA	2.50	0.59
1:A:472:GLN:O	1:A:472:GLN:HG3	2.02	0.59
1:B:483:ARG:CB	1:B:483:ARG:HH11	2.15	0.59
1:A:450:ASP:HB3	1:A:508:LEU:HD22	1.83	0.59
1:B:240:VAL:O	1:B:241[B]:GLU:CA	2.51	0.59
1:B:472:GLN:OE1	2:B:1531:ACT:CH3	2.51	0.59
1:B:432:ARG:CG	1:B:432:ARG:HH11	2.16	0.58
1:B:381:LEU:HD22	1:B:385:ARG:HH11	1.69	0.58
1:A:173:ARG:HD2	1:B:112:THR:HG22	1.86	0.58
1:B:74:ARG:NH1	1:B:124:GLY:HA3	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:O	1:B:42:GLU:N	2.36	0.57
1:A:438:VAL:HG12	1:A:453:VAL:HG11	1.85	0.57
1:B:169:GLY:O	1:B:172:GLY:N	2.27	0.57
1:B:38:HIS:CD2	1:B:43:LYS:HD3	2.40	0.56
1:A:304:ARG:HG3	1:A:304:ARG:NH1	2.21	0.56
1:A:189:GLU:O	1:A:192:SER:HB2	2.05	0.56
1:B:327:GLU:OE1	1:B:327:GLU:HA	2.05	0.56
1:A:123:PRO:O	1:A:125:ASP:N	2.38	0.56
1:B:155:ARG:HB2	1:B:156:PRO:HD2	1.88	0.56
1:A:423:ASP:N	1:A:423:ASP:OD1	2.39	0.56
1:A:127:PRO:C	1:A:128:GLU:CG	2.71	0.55
1:A:243:ALA:O	1:A:246:VAL:HG12	2.06	0.55
1:A:450:ASP:HB3	1:A:508:LEU:CD2	2.37	0.55
1:A:127:PRO:O	1:A:128:GLU:OE2	2.24	0.54
1:B:56:LEU:CD1	1:B:142:LEU:HD22	2.36	0.54
1:B:75:MET:SD	1:B:136:GLU:HG3	2.48	0.54
1:B:459:ALA:HB1	1:B:460:PRO:HD2	1.89	0.54
1:B:56:LEU:HD12	1:B:142:LEU:HD22	1.90	0.54
1:B:171:THR:OG1	1:B:173:ARG:HB2	2.07	0.53
1:A:85:MET:HA	1:A:88:ILE:HD12	1.91	0.53
1:A:19:THR:HG22	1:A:20:LEU:N	2.24	0.53
1:B:75:MET:HE3	1:B:81:ALA:HA	1.91	0.53
1:B:389:GLY:C	1:B:399:PRO:HD2	2.29	0.53
1:B:486:ARG:O	1:B:490:LYS:HD2	2.08	0.53
1:A:265:THR:HG22	1:A:269:LEU:HD22	1.91	0.53
1:A:59:LEU:O	1:A:59:LEU:HD23	2.09	0.53
1:A:127:PRO:O	1:A:128:GLU:HG3	2.07	0.53
1:A:19:THR:HG22	1:A:21:VAL:H	1.74	0.52
1:B:38:HIS:CG	1:B:249:ARG:NH1	2.77	0.52
1:B:123:PRO:CD	1:B:124:GLY:N	2.73	0.52
1:B:19:THR:HG23	1:B:181:HIS:ND1	2.25	0.52
1:B:427:LYS:HD2	1:B:432:ARG:HH21	1.74	0.52
1:B:241[A]:GLU:HA	1:B:244:ARG:HD3	1.92	0.51
1:B:38:HIS:CD2	1:B:43:LYS:CD	2.94	0.51
1:B:204:LEU:HD23	1:B:254:LEU:CD1	2.41	0.51
1:A:358:THR:HG23	1:A:410:ARG:O	2.10	0.51
1:B:294:ARG:N	1:B:295:PRO:CD	2.74	0.50
1:B:472:GLN:OE1	2:B:1531:ACT:H1	2.11	0.50
1:B:106:ARG:O	1:B:110:ILE:HG13	2.11	0.50
1:B:19:THR:HG22	1:B:21:VAL:H	1.75	0.50
1:A:183:ASN:HB3	1:A:317:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ALA:O	1:A:360:GLU:HB3	2.12	0.50
1:B:38:HIS:CG	1:B:249:ARG:HH12	2.29	0.50
1:A:288:LEU:O	1:A:335:SER:OG	2.30	0.50
1:A:161:VAL:HA	1:A:180:ARG:HA	1.93	0.49
1:B:456:HIS:O	1:B:463:SER:HA	2.11	0.49
1:A:510:ARG:HD3	1:A:514:GLY:O	2.12	0.49
1:A:282:VAL:HG22	1:A:308:ILE:HG13	1.95	0.49
1:B:241[B]:GLU:HA	1:B:244:ARG:HD3	1.93	0.49
1:B:425:GLN:HG3	1:B:434:GLU:OE1	2.13	0.49
1:A:326:THR:CG2	1:A:327:GLU:N	2.71	0.49
1:B:483:ARG:HG3	1:B:483:ARG:NH1	2.27	0.49
1:B:483:ARG:CG	1:B:483:ARG:NH1	2.73	0.49
1:B:348:ILE:HG22	1:B:362:GLY:HA3	1.95	0.48
1:B:170:THR:HG21	1:B:423:ASP:OD2	2.13	0.48
1:A:289:THR:O	1:A:292:VAL:CG2	2.62	0.48
1:B:174:PRO:HB3	1:B:512:ILE:HG12	1.94	0.48
1:A:407:LEU:N	1:A:420:GLY:O	2.36	0.47
1:B:145:ARG:CG	1:B:145:ARG:NH1	2.72	0.47
1:B:483:ARG:HG3	1:B:483:ARG:HH11	1.78	0.47
1:B:170:THR:HG21	1:B:423:ASP:CB	2.45	0.47
1:B:20:LEU:HD21	1:B:184:VAL:HG11	1.96	0.47
1:B:122:ASP:HB2	1:B:123:PRO:CD	2.44	0.47
1:B:48:LEU:HD11	1:B:143:ARG:O	2.14	0.47
1:B:344:PHE:HA	1:B:367:ALA:O	2.15	0.47
1:B:211:PHE:N	1:B:211:PHE:CD1	2.81	0.47
1:A:326:THR:CG2	1:A:327:GLU:H	2.18	0.47
1:B:313:ILE:HD12	1:B:402:TYR:CE2	2.49	0.47
1:B:240:VAL:O	1:B:241[A]:GLU:HA	2.15	0.47
1:B:427:LYS:HD2	1:B:432:ARG:CZ	2.45	0.47
1:B:80:ASN:HD22	1:B:136:GLU:HG2	1.80	0.46
1:A:99:ASP:O	1:A:102:ASN:HB2	2.15	0.46
1:A:289:THR:O	1:A:292:VAL:HG22	2.15	0.46
1:B:39:ILE:O	1:B:42:GLU:CB	2.64	0.46
1:B:518:ARG:HA	1:B:521:VAL:HG12	1.98	0.46
1:A:348:ILE:HG22	1:A:362:GLY:HA3	1.96	0.46
1:B:483:ARG:HH11	1:B:483:ARG:HB2	1.81	0.46
1:B:39:ILE:O	1:B:40:ASP:C	2.53	0.45
1:A:123:PRO:HG3	1:A:133:LEU:HD11	1.98	0.45
1:A:326:THR:HB	1:A:328:ASP:OD1	2.15	0.45
1:B:313:ILE:HG13	1:B:316:THR:OG1	2.16	0.45
1:B:14:SER:HB3	1:B:17:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:O	1:A:128:GLU:CG	2.65	0.45
1:A:246:VAL:HG23	1:A:251:ILE:HB	1.99	0.45
1:A:57:ALA:HB2	1:A:90:ARG:HB3	1.98	0.45
1:A:456:HIS:HE1	1:A:526:ASP:OD1	1.98	0.45
1:A:166:TYR:HA	1:A:175:LYS:O	2.16	0.45
1:B:406:ASP:CG	1:B:421:ARG:HE	2.20	0.45
1:A:438:VAL:HB	1:A:453:VAL:HG21	1.97	0.44
1:B:145:ARG:HG2	1:B:145:ARG:NH1	2.32	0.44
1:B:19:THR:HG22	1:B:20:LEU:N	2.33	0.44
1:A:373:GLU:O	1:A:400:ARG:NH2	2.50	0.44
1:A:359:GLY:O	1:A:361:PRO:HD3	2.18	0.44
1:B:432:ARG:CG	1:B:432:ARG:NH1	2.73	0.44
1:A:435:LEU:HA	1:A:435:LEU:HD23	1.87	0.44
1:B:136:GLU:O	1:B:139:VAL:CG2	2.64	0.44
1:B:263:ALA:HA	2:B:1531:ACT:H2	2.00	0.44
1:A:465:LEU:HB3	1:A:499:PRO:HA	2.00	0.44
1:B:298:LYS:HA	1:B:298:LYS:HD2	1.51	0.44
1:A:524:ALA:O	1:A:528:ARG:HG3	2.17	0.43
1:B:459:ALA:HB3	1:B:462:ASP:HB3	2.00	0.43
1:A:304:ARG:CG	1:A:304:ARG:NH1	2.79	0.43
1:A:518:ARG:HG3	1:A:518:ARG:NH1	2.32	0.43
1:B:19:THR:HG23	1:B:181:HIS:CG	2.53	0.43
1:B:122:ASP:HB2	1:B:123:PRO:HD2	1.99	0.43
1:B:263:ALA:HA	1:B:472:GLN:OE1	2.18	0.43
1:A:244:ARG:NH1	1:A:271:GLU:OE1	2.52	0.43
1:A:513:ASN:OD1	1:A:513:ASN:N	2.41	0.43
1:B:204:LEU:HD23	1:B:254:LEU:HD13	2.00	0.43
1:B:315:GLU:O	1:B:372:SER:HB3	2.19	0.43
1:B:240:VAL:O	1:B:241[B]:GLU:HA	2.18	0.43
1:A:59:LEU:C	1:A:59:LEU:HD23	2.40	0.42
1:B:127:PRO:HD2	1:B:128:GLU:H	1.84	0.42
1:B:189:GLU:O	1:B:192:SER:HB2	2.18	0.42
1:B:364:LEU:O	1:B:404:SER:HB2	2.18	0.42
1:B:218:ILE:O	1:B:222:LEU:HB2	2.18	0.42
1:B:60:LEU:O	1:B:65:VAL:HG13	2.20	0.42
1:A:19:THR:HG23	1:A:181:HIS:ND1	2.33	0.42
1:A:332:ALA:HB3	3:A:2030:HOH:O	2.19	0.42
1:B:452:VAL:HG23	1:B:468:ALA:HB3	2.01	0.42
1:A:19:THR:HG23	1:A:181:HIS:CG	2.54	0.42
1:A:308:ILE:HD12	1:A:308:ILE:C	2.40	0.42
1:B:306:HIS:CD2	1:B:324:ARG:HH11	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD11	1:A:281:VAL:HG22	2.01	0.42
1:B:144:ASP:OD1	1:B:144:ASP:N	2.49	0.42
1:A:287:LYS:HG3	1:A:418:TYR:CD2	2.55	0.42
1:A:524:ALA:O	1:A:528:ARG:CG	2.68	0.42
1:B:169:GLY:C	1:B:171:THR:N	2.71	0.42
1:B:364:LEU:O	1:B:404:SER:CB	2.68	0.42
1:A:211:PHE:CZ	1:A:213:PHE:HB2	2.55	0.41
1:A:519:ALA:O	1:A:523:ARG:HG3	2.20	0.41
1:A:99:ASP:OD2	1:A:101:ARG:HB2	2.20	0.41
1:B:201:ASP:O	1:B:226:ALA:HB1	2.20	0.41
1:A:19:THR:CG2	1:A:20:LEU:N	2.82	0.41
1:A:277:GLU:HB2	3:A:2018:HOH:O	2.21	0.41
1:A:294:ARG:N	1:A:295:PRO:CD	2.82	0.41
1:A:88:ILE:HG21	1:A:95:TYR:HB3	2.02	0.41
1:B:304:ARG:HA	1:B:305:PRO:HA	1.87	0.41
1:B:458:PHE:CE1	1:B:464:ARG:CG	3.03	0.41
1:A:109:PHE:CE2	1:A:174:PRO:HG2	2.55	0.41
1:B:318:VAL:HG12	1:B:319:HIS:CE1	2.55	0.41
1:B:39:ILE:HD13	1:B:230:VAL:HB	2.02	0.41
1:B:458:PHE:CE1	1:B:464:ARG:HG2	2.56	0.41
1:A:102:ASN:CG	1:A:106:ARG:HD3	2.41	0.41
1:A:78:GLY:O	1:A:82:ILE:HD12	2.21	0.41
1:B:360:GLU:HA	1:B:361:PRO:HD2	1.97	0.41
1:A:459:ALA:HB1	1:A:460:PRO:CD	2.51	0.40
1:B:136:GLU:HA	1:B:139:VAL:HG22	2.03	0.40
1:B:318:VAL:HG12	1:B:319:HIS:ND1	2.35	0.40
1:B:398:PRO:HA	1:B:399:PRO:HD3	1.94	0.40
1:B:386:PHE:HA	1:B:401:TYR:O	2.20	0.40
1:B:39:ILE:CD1	1:B:230:VAL:HG21	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:O	1:B:196:SER:OG[3_445]	2.15	0.05

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	477/529 (90%)	470 (98%)	6 (1%)	1 (0%)	52 64
1	B	489/529 (92%)	481 (98%)	8 (2%)	0	100 100
All	All	966/1058 (91%)	951 (98%)	14 (1%)	1 (0%)	56 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	PRO

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	389/420 (93%)	329 (85%)	60 (15%)	3 2
1	B	398/420 (95%)	352 (88%)	46 (12%)	7 7
All	All	787/840 (94%)	681 (86%)	106 (14%)	5 4

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	21	VAL
1	A	23	LEU
1	A	26	ARG
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	41	ASP
1	A	42	GLU
1	A	56	LEU
1	A	65	VAL
1	A	70	ARG
1	A	89	LEU
1	A	90	ARG
1	A	98	LEU
1	A	112	THR
1	A	116	VAL
1	A	119	LEU
1	A	133	LEU
1	A	137	GLU
1	A	145	ARG
1	A	161	VAL
1	A	167	THR
1	A	173	ARG
1	A	175	LYS
1	A	194	LEU
1	A	202	ARG
1	A	212	ASP
1	A	213	PHE
1	A	232	PRO
1	A	245	VAL
1	A	247	ARG
1	A	269	LEU
1	A	278	LEU
1	A	286	GLU
1	A	287	LYS
1	A	292	VAL
1	A	299	ARG
1	A	307	LEU
1	A	308	ILE
1	A	313	ILE
1	A	314	THR
1	A	335	SER
1	A	351	GLU
1	A	380	GLU
1	A	385	ARG
1	A	403	HIS
1	A	404	SER
1	A	409	SER

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Mol	Chain	Res	Type
1	A	421	ARG
1	A	423	ASP
1	A	427	LYS
1	A	450	ASP
1	A	452	VAL
1	A	483	ARG
1	A	486	ARG
1	A	495	SER
1	A	508	LEU
1	A	513	ASN
1	A	518	ARG
1	A	521	VAL
1	A	528	ARG
1	B	25	SER
1	B	26	ARG
1	B	39	ILE
1	B	43	LYS
1	B	51	SER
1	B	56	LEU
1	B	65	VAL
1	B	74	ARG
1	B	85	MET
1	B	98	LEU
1	B	119	LEU
1	B	126	ILE
1	B	130	THR
1	B	145	ARG
1	B	146	GLU
1	B	167	THR
1	B	170	THR
1	B	192	SER
1	B	194	LEU
1	B	196	SER
1	B	213	PHE
1	B	222	LEU
1	B	237	ARG
1	B	238	THR
1	B	244	ARG
1	B	298	LYS
1	B	299	ARG
1	B	330	LEU
1	B	335	SER

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Mol	Chain	Res	Type
1	B	341	LEU
1	B	351	GLU
1	B	372	SER
1	B	410	ARG
1	B	419	GLN
1	B	421	ARG
1	B	428	LEU
1	B	435	LEU
1	B	452	VAL
1	B	464	ARG
1	B	465	LEU
1	B	472	GLN
1	B	483	ARG
1	B	495	SER
1	B	508	LEU
1	B	512	ILE
1	B	529	ARG

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

Mol	Chain	Res	Type
1	A	306	HIS
1	A	456	HIS
1	A	472	GLN
1	B	80	ASN
1	B	306	HIS

5.3.3 RNA (i)

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)

3 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	ACT	A	1530	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	B	1530	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ACT	B	1531	-	0,3,3	0.00	-	0,3,3	0.00	-

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	ACT	A	1530	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1530	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1531	-	-	0/0/0/0	0/0/0/0

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1531	ACT	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	488/529 (92%)	0.05	12 (2%)	61	63	16, 36, 59, 81	0
1	B	496/529 (93%)	0.08	14 (2%)	56	60	19, 35, 65, 97	0
All	All	984/1058 (93%)	0.07	26 (2%)	59	62	16, 36, 63, 97	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	SER	5.6
1	B	40	ASP	5.3
1	A	125	ASP	4.6
1	B	460	PRO	4.1
1	B	430	GLY	4.0
1	A	478	THR	3.6
1	A	473	ALA	3.6
1	A	398	PRO	3.2
1	B	129	TYR	3.1
1	A	389	GLY	3.1
1	B	389	GLY	2.8
1	B	169	GLY	2.6
1	B	146	GLU	2.6
1	A	130	THR	2.6
1	A	429	ARG	2.5
1	B	128	GLU	2.4
1	A	388	THR	2.4
1	B	397	PRO	2.3
1	B	144	ASP	2.3
1	A	172	GLY	2.2
1	B	127	PRO	2.2
1	B	170	THR	2.2
1	A	127	PRO	2.1
1	B	237	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	460	PRO	2.0
1	A	146	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	ACT	B	1531	4/4	0.75	0.34	6.18	53,53,54,54	0
2	ACT	A	1530	4/4	0.93	0.21	2.07	55,55,55,56	0
2	ACT	B	1530	4/4	0.96	0.12	-0.93	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.