



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:48 AM GMT

PDB ID : 3Q35  
Title : Structure of the Rtt109-AcCoA/Vps75 complex and implications for  
chaperone-mediated histone acetylation  
Authors : Tang, Y.; Yuan, H.; Meeth, K.; Marmorstein, R.  
Deposited on : 2010-12-21  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

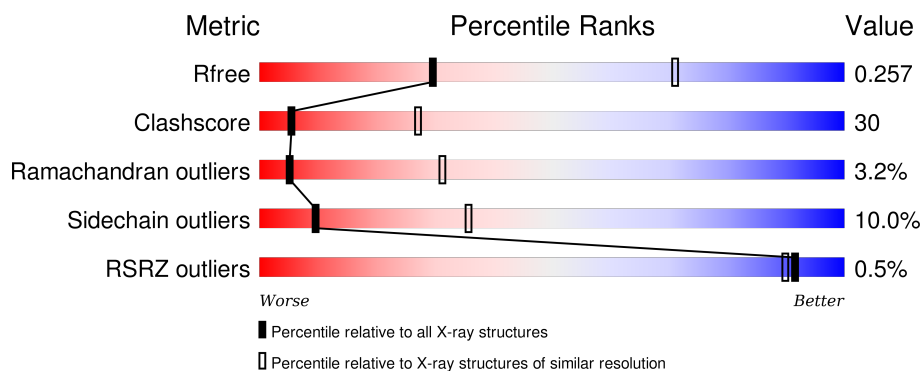
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	438	
2	B	232	

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
1	ALY	A	290	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5040 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 Histone acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3198	2058	539	592	9			

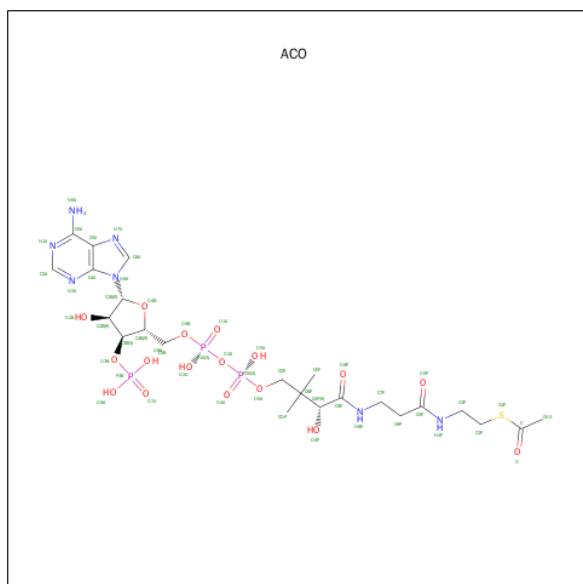
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q07794
A	0	SER	-	EXPRESSION TAG	UNP Q07794

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 75.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1776	1149	288	334	5			

- Molecule 3 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	2	Total	O	0	0
			2	2		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.08 Å 119.00 Å 80.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 3.30 47.80 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.01-3.30) 99.8 (47.80-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 3.33 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.207 , 0.248 0.215 , 0.257	Depositor DCC
$R_{free}$ test set	739 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14672 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: ACO, EDO, ALY

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	0.55	0/3255	0.66	0/4402
2	B	0.52	0/1823	0.64	0/2455
All	All	0.54	0/5078	0.66	0/6857

There are no bond length outliers.

There are no bond angle outliers.

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	3198	0	3239	196	0
2	B	1776	0	1721	104	0
3	A	51	0	34	3	0
4	A	4	0	6	2	0
5	A	9	0	0	1	0
5	B	2	0	0	0	0
All	All	5040	0	5000	299	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 30.

All (299) 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:B:164:ARG:HH11	2:B:164:ARG:HG3	1.21	0.99
1:A:238:THR:HG23	1:A:334:GLY:HA3	1.49	0.92
2:B:10:GLU:OE2	2:B:13:LYS:HD2	1.70	0.92
1:A:115:ASP:HB2	1:A:341:SER:HA	1.48	0.91
1:A:13:VAL:HA	1:A:400:GLY:O	1.70	0.91
1:A:138:ILE:HD13	1:A:147:THR:HG23	1.49	0.91
2:B:184:ARG:HG3	2:B:184:ARG:HH11	1.40	0.86
1:A:298:ALA:HA	1:A:303:LEU:HD21	1.57	0.84
1:A:262:PRO:HB2	1:A:263:LEU:HD13	1.60	0.84
1:A:319:GLN:HA	1:A:322:LYS:HB3	1.61	0.82
2:B:164:ARG:HH11	2:B:164:ARG:CG	1.93	0.81
1:A:288:ASP:OD2	1:A:290:ALY:HB3	1.82	0.80
1:A:118:TYR:CE1	1:A:344:PRO:HD2	2.18	0.79
1:A:247:GLU:OE1	1:A:251:ARG:HD3	1.83	0.77
2:B:25:VAL:HA	2:B:28:ILE:HD12	1.69	0.74
1:A:105:LYS:HB2	1:A:225:ILE:HG23	1.70	0.73
1:A:16:GLN:HA	1:A:398:LEU:O	1.89	0.73
1:A:101:ARG:HB2	1:A:221:TRP:NE1	2.04	0.72
2:B:129:LYS:HD2	2:B:129:LYS:H	1.55	0.72
1:A:214:ASN:OD1	1:A:217:GLU:HG3	1.91	0.71
2:B:189:LYS:HD2	2:B:189:LYS:N	2.06	0.71
2:B:164:ARG:NH1	2:B:164:ARG:HG3	1.94	0.70
1:A:303:LEU:H	1:A:303:LEU:HD12	1.55	0.70
1:A:384:ARG:HG3	1:A:385:ASP:H	1.56	0.70
2:B:155:ILE:HD12	2:B:175:GLY:HA2	1.74	0.70
2:B:179:ILE:O	2:B:179:ILE:HD13	1.92	0.70
2:B:78:LYS:HD3	2:B:79:TYR:CE1	2.27	0.69
1:A:304:LEU:N	1:A:304:LEU:HD12	2.07	0.69
1:A:101:ARG:HB2	1:A:221:TRP:HE1	1.58	0.69
2:B:94:GLU:O	2:B:95:SER:HB3	1.93	0.69
1:A:319:GLN:O	1:A:321:PHE:N	2.26	0.68
2:B:46:LYS:O	2:B:49:ALA:HB3	1.93	0.68
1:A:154:ARG:NH2	1:A:163:LEU:HD11	2.09	0.68
1:A:384:ARG:HG3	1:A:385:ASP:N	2.07	0.68
1:A:37:LYS:HB3	1:A:37:LYS:NZ	2.10	0.67
2:B:184:ARG:CG	2:B:184:ARG:HH11	2.06	0.67
2:B:105:ILE:HG22	2:B:107:PHE:CE2	2.30	0.67
1:A:1:MET:HB2	1:A:5:ASP:OD2	1.95	0.67
1:A:154:ARG:CZ	1:A:163:LEU:HD11	2.25	0.66
1:A:86:SER:O	4:A:437:EDO:H12	1.95	0.66
1:A:293:PHE:HD2	1:A:315:LEU:HD13	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD21	1:A:312:TRP:HE1	1.60	0.65
1:A:235:GLN:HG3	1:A:335:TYR:O	1.96	0.65
1:A:125:PRO:HG3	1:A:177:LEU:HG	1.78	0.65
1:A:193:THR:O	1:A:194:ARG:HG3	1.97	0.65
1:A:28:GLU:O	1:A:28:GLU:HG2	1.97	0.65
1:A:292:ARG:NH1	1:A:320:GLU:HG2	2.12	0.65
1:A:186:LEU:HD12	1:A:334:GLY:O	1.97	0.64
1:A:122:LYS:HE3	1:A:176:TYR:HB3	1.79	0.64
2:B:218:GLU:O	2:B:221:ARG:HG2	1.97	0.64
2:B:102:ASP:OD1	2:B:126:GLN:HA	1.98	0.63
1:A:248:ASP:O	1:A:251:ARG:HB2	1.98	0.63
1:A:318:ARG:HH11	1:A:318:ARG:HG3	1.62	0.63
1:A:184:GLU:HB2	1:A:339:THR:HG23	1.81	0.63
2:B:77:PHE:HA	2:B:80:ILE:HB	1.81	0.62
1:A:13:VAL:HG12	1:A:401:LYS:HA	1.80	0.62
1:A:247:GLU:HG3	1:A:248:ASP:H	1.64	0.62
1:A:191:LEU:C	1:A:191:LEU:HD12	2.20	0.62
1:A:365:ILE:HG22	1:A:366:THR:N	2.15	0.61
1:A:44:LYS:HB3	1:A:73:LEU:O	1.99	0.61
2:B:156:ASN:HB3	2:B:159:LEU:HB2	1.82	0.60
1:A:270:PHE:HZ	1:A:290:ALY:HH32	1.66	0.60
2:B:90:TRP:HD1	2:B:103:PHE:HB3	1.66	0.60
2:B:84:ASP:OD2	2:B:110:HIS:HB3	2.02	0.60
1:A:243:ARG:NH1	1:A:268:ASP:OD2	2.35	0.60
1:A:115:ASP:HB2	1:A:341:SER:CA	2.29	0.60
1:A:18:GLU:O	1:A:56:PHE:N	2.32	0.60
1:A:298:ALA:CA	1:A:303:LEU:HD21	2.32	0.60
1:A:308:LEU:CD2	1:A:312:TRP:HE1	2.15	0.60
2:B:30:ARG:NH2	2:B:96:GLU:HA	2.17	0.59
1:A:270:PHE:HZ	1:A:290:ALY:CH3	2.15	0.59
2:B:184:ARG:CG	2:B:184:ARG:NH1	2.64	0.59
2:B:25:VAL:HA	2:B:28:ILE:CD1	2.31	0.59
1:A:46:THR:C	1:A:47:ILE:HD12	2.23	0.59
2:B:221:ARG:NH1	2:B:221:ARG:HG3	2.16	0.58
1:A:109:GLU:O	1:A:112:LEU:HB2	2.03	0.58
2:B:103:PHE:C	2:B:103:PHE:CD1	2.77	0.58
2:B:162:ASP:O	2:B:168:GLY:HA3	2.04	0.58
1:A:318:ARG:O	1:A:320:GLU:OE2	2.22	0.57
2:B:188:LEU:C	2:B:189:LYS:HD2	2.25	0.57
1:A:181:CYS:HB2	1:A:182:PRO:HD2	1.86	0.57
1:A:245:PRO:HD2	1:A:327:SER:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLU:HB3	1:A:370:TYR:CE2	2.40	0.57
1:A:82:LEU:C	1:A:82:LEU:HD23	2.25	0.57
1:A:136:GLU:OE1	1:A:153:ARG:HD2	2.04	0.56
2:B:195:PRO:O	2:B:196:HIS:HB2	2.05	0.56
2:B:222:ASP:O	2:B:223:LEU:HB2	2.06	0.56
2:B:110:HIS:HA	2:B:118:GLU:HG2	1.87	0.56
1:A:199:TYR:HE1	3:A:999:ACO:H32	1.70	0.56
2:B:209:TYR:HB3	2:B:210:PRO:HD3	1.88	0.56
2:B:119:GLN:OE1	2:B:146:ILE:HG13	2.06	0.56
2:B:173:ARG:HG3	2:B:173:ARG:HH11	1.69	0.55
1:A:45:SER:OG	1:A:73:LEU:HD12	2.06	0.55
2:B:105:ILE:CG2	2:B:107:PHE:CE2	2.89	0.55
1:A:151:LEU:HD11	2:B:220:GLN:HG2	1.88	0.55
2:B:25:VAL:HA	2:B:28:ILE:CG1	2.36	0.55
2:B:179:ILE:O	2:B:182:TRP:HB3	2.07	0.55
1:A:318:ARG:O	1:A:319:GLN:HG3	2.06	0.55
1:A:149:ARG:HG3	1:A:149:ARG:HH11	1.72	0.55
2:B:65:HIS:CE1	2:B:67:SER:HB3	2.42	0.55
2:B:189:LYS:HB3	2:B:192:LYS:HB2	1.88	0.55
1:A:47:ILE:N	1:A:47:ILE:HD12	2.22	0.54
1:A:378:GLU:HA	1:A:378:GLU:OE2	2.06	0.54
1:A:13:VAL:HA	1:A:400:GLY:C	2.28	0.54
1:A:106:ILE:HG22	1:A:107:ILE:N	2.22	0.54
1:A:318:ARG:HB2	1:A:318:ARG:CZ	2.37	0.54
1:A:299:GLU:C	1:A:301:ASP:H	2.10	0.54
1:A:228:ARG:O	1:A:232:GLU:HG3	2.07	0.54
1:A:68:TYR:CE2	1:A:286:PRO:HG2	2.43	0.54
2:B:24:GLU:O	2:B:28:ILE:HG13	2.08	0.54
1:A:6:PHE:HB3	1:A:106:ILE:HG23	1.89	0.54
1:A:304:LEU:HD12	1:A:304:LEU:H	1.72	0.54
1:A:294:ILE:HG22	1:A:295:HIS:N	2.23	0.54
1:A:344:PRO:HB3	1:A:348:ASP:HB3	1.90	0.53
1:A:248:ASP:O	1:A:251:ARG:N	2.41	0.53
1:A:298:ALA:HA	1:A:303:LEU:CD2	2.32	0.53
2:B:221:ARG:HG3	2:B:221:ARG:HH11	1.72	0.53
2:B:99:ASP:N	2:B:102:ASP:OD2	2.40	0.53
1:A:302:ARG:NH2	1:A:314:GLU:OE1	2.42	0.53
1:A:293:PHE:HD2	1:A:315:LEU:CD1	2.22	0.53
1:A:67:VAL:HG13	1:A:84:PHE:O	2.08	0.53
1:A:123:VAL:O	1:A:125:PRO:HD3	2.09	0.52
2:B:83:ILE:HG22	2:B:83:ILE:O	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ARG:NH1	2:B:164:ARG:CG	2.63	0.52
1:A:195:PRO:HD2	5:A:442:HOH:O	2.10	0.52
1:A:59:GLY:HA2	1:A:380:PHE:CD2	2.44	0.52
1:A:225:ILE:O	1:A:229:LEU:HG	2.10	0.52
1:A:144:PRO:O	1:A:148:LEU:HG	2.10	0.52
2:B:38:ASN:OD1	2:B:93:LEU:HD22	2.10	0.52
1:A:41:ARG:HD2	1:A:74:TRP:HB3	1.91	0.52
2:B:94:GLU:O	2:B:95:SER:CB	2.58	0.51
1:A:163:LEU:N	1:A:163:LEU:HD12	2.26	0.51
1:A:37:LYS:HB3	1:A:37:LYS:HZ2	1.75	0.51
1:A:155:LEU:O	1:A:158:SER:O	2.28	0.51
1:A:357:GLN:HE22	1:A:391:MET:HG2	1.75	0.51
1:A:109:GLU:HA	1:A:112:LEU:HD12	1.92	0.51
1:A:261:TYR:HB3	1:A:264:TRP:CD1	2.45	0.51
1:A:124:LYS:HZ2	1:A:128:ARG:HH22	1.59	0.51
2:B:25:VAL:HG22	2:B:28:ILE:HD12	1.92	0.51
1:A:20:LEU:O	1:A:53:PHE:HA	2.11	0.51
1:A:293:PHE:CD2	1:A:315:LEU:HD13	2.45	0.50
1:A:357:GLN:O	1:A:361:ILE:HG13	2.11	0.50
1:A:115:ASP:H	1:A:342:LEU:H	1.58	0.50
1:A:401:LYS:HG3	1:A:401:LYS:O	2.12	0.50
2:B:123:LYS:HE3	2:B:141:SER:OG	2.12	0.50
1:A:36:ASN:HD21	1:A:39:ASP:CG	2.15	0.50
1:A:212:ILE:N	1:A:212:ILE:HD12	2.27	0.50
1:A:6:PHE:HB3	1:A:106:ILE:CG2	2.41	0.50
1:A:318:ARG:HH11	1:A:318:ARG:CG	2.24	0.49
1:A:342:LEU:O	1:A:344:PRO:HD3	2.12	0.49
1:A:124:LYS:NZ	1:A:128:ARG:HH12	2.11	0.49
1:A:372:THR:C	1:A:374:GLU:H	2.14	0.49
1:A:350:ILE:O	1:A:352:PRO:HD3	2.11	0.49
2:B:110:HIS:HD1	2:B:110:HIS:C	2.15	0.49
2:B:152:TYR:N	2:B:152:TYR:CD1	2.80	0.49
2:B:211:PHE:O	2:B:213:VAL:N	2.46	0.49
1:A:282:ILE:HG23	1:A:290:ALY:HD3	1.94	0.49
2:B:189:LYS:HB3	2:B:192:LYS:HD2	1.94	0.49
2:B:76:ASP:O	2:B:80:ILE:HG13	2.13	0.49
2:B:117:LYS:HE3	2:B:147:GLU:OE2	2.13	0.49
2:B:36:ARG:O	2:B:40:MET:HG2	2.13	0.49
1:A:60:LYS:NZ	1:A:373:GLU:OE1	2.43	0.49
2:B:29:GLU:HA	2:B:32:VAL:HG22	1.95	0.48
1:A:28:GLU:O	1:A:28:GLU:CG	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:HG3	1:A:317:GLU:OE1	2.13	0.48
1:A:325:VAL:HG12	1:A:326:THR:H	1.78	0.48
2:B:143:PRO:HD3	2:B:186:THR:HG22	1.94	0.48
2:B:95:SER:C	2:B:97:MET:H	2.16	0.48
1:A:293:PHE:CD2	1:A:315:LEU:CD1	2.96	0.48
1:A:293:PHE:HE1	1:A:297:LEU:HD21	1.78	0.48
1:A:6:PHE:HD2	1:A:106:ILE:HD12	1.78	0.48
2:B:151:SER:C	2:B:153:ASP:H	2.16	0.48
2:B:189:LYS:O	2:B:190:PRO:C	2.51	0.48
1:A:13:VAL:C	1:A:15:GLU:H	2.16	0.47
2:B:110:HIS:ND1	2:B:110:HIS:C	2.67	0.47
2:B:110:HIS:ND1	2:B:110:HIS:O	2.45	0.47
3:A:999:ACO:O2A	3:A:999:ACO:O5A	2.33	0.47
1:A:59:GLY:HA2	1:A:380:PHE:CE2	2.49	0.47
2:B:37:LEU:HD13	2:B:90:TRP:CB	2.44	0.47
1:A:353:LYS:HG3	1:A:354:SER:HB3	1.96	0.47
1:A:12:PRO:O	1:A:15:GLU:HB2	2.13	0.47
1:A:372:THR:C	1:A:374:GLU:N	2.67	0.47
1:A:75:ASP:C	1:A:75:ASP:OD1	2.51	0.47
1:A:122:LYS:CE	1:A:176:TYR:HB3	2.44	0.47
2:B:80:ILE:O	2:B:83:ILE:HG13	2.14	0.47
2:B:72:ILE:O	2:B:72:ILE:HG13	2.12	0.47
1:A:277:LEU:HD21	1:A:304:LEU:HA	1.97	0.47
1:A:136:GLU:HA	1:A:136:GLU:OE2	2.15	0.47
1:A:249:PRO:O	1:A:253:ARG:HG3	2.15	0.47
1:A:13:VAL:HG13	1:A:402:ARG:N	2.30	0.46
1:A:263:LEU:O	1:A:265:GLN:HG3	2.15	0.46
1:A:120:LEU:HD22	1:A:179:PHE:HB2	1.96	0.46
1:A:193:THR:HG22	1:A:222:TRP:CD1	2.50	0.46
2:B:84:ASP:OD2	2:B:108:HIS:ND1	2.48	0.46
1:A:352:PRO:HA	1:A:391:MET:HE3	1.97	0.46
1:A:118:TYR:CD1	1:A:344:PRO:HD2	2.50	0.46
1:A:214:ASN:OD1	1:A:217:GLU:CG	2.61	0.46
2:B:58:TRP:HB2	2:B:83:ILE:O	2.15	0.46
1:A:62:PHE:HA	1:A:91:ASN:OD1	2.16	0.46
2:B:86:ILE:HA	2:B:106:THR:O	2.15	0.46
2:B:20:LYS:O	2:B:24:GLU:HG3	2.15	0.46
1:A:17:PHE:O	1:A:18:GLU:HG3	2.15	0.46
1:A:263:LEU:N	1:A:263:LEU:CD1	2.79	0.46
1:A:357:GLN:O	1:A:360:ALA:HB3	2.16	0.46
1:A:372:THR:O	1:A:374:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:C	1:A:163:LEU:HD12	2.36	0.45
1:A:162:VAL:HG12	1:A:163:LEU:H	1.81	0.45
1:A:200:LEU:O	1:A:366:THR:HA	2.17	0.45
1:A:322:LYS:O	1:A:323:LEU:HD23	2.16	0.45
1:A:3:LEU:O	1:A:6:PHE:HB2	2.16	0.45
2:B:141:SER:O	2:B:186:THR:HG22	2.16	0.45
1:A:293:PHE:O	1:A:296:GLN:HB2	2.17	0.45
1:A:194:ARG:NH1	4:A:437:EDO:O2	2.43	0.45
1:A:271:THR:HG22	1:A:272:SER:N	2.32	0.45
1:A:318:ARG:C	1:A:319:GLN:HG3	2.38	0.45
1:A:332:ILE:CG2	1:A:333:SER:N	2.80	0.45
1:A:308:LEU:CD2	1:A:312:TRP:NE1	2.79	0.44
1:A:302:ARG:HH22	1:A:314:GLU:CD	2.20	0.44
2:B:189:LYS:N	2:B:189:LYS:CD	2.80	0.44
1:A:89:ASP:OD2	1:A:199:TYR:N	2.41	0.44
1:A:228:ARG:NE	1:A:232:GLU:OE2	2.50	0.44
1:A:248:ASP:HB3	1:A:251:ARG:CG	2.47	0.44
1:A:293:PHE:CE1	1:A:297:LEU:HD21	2.53	0.44
1:A:261:TYR:CE2	1:A:263:LEU:HB2	2.53	0.44
1:A:270:PHE:CZ	1:A:290:ALY:CH3	2.99	0.44
2:B:204:PHE:HA	2:B:208:ILE:HB	2.00	0.44
2:B:21:CYS:O	2:B:25:VAL:HG23	2.18	0.44
1:A:398:LEU:HA	1:A:398:LEU:HD23	1.76	0.44
1:A:120:LEU:HB3	1:A:179:PHE:O	2.18	0.43
1:A:303:LEU:HB2	1:A:304:LEU:HD12	2.00	0.43
1:A:261:TYR:HA	1:A:262:PRO:HD3	1.67	0.43
2:B:159:LEU:HD22	2:B:159:LEU:HA	1.67	0.43
1:A:242:LEU:HG	1:A:243:ARG:N	2.33	0.43
1:A:19:TYR:HB2	1:A:55:LEU:HD12	2.00	0.43
1:A:122:LYS:HD3	1:A:176:TYR:HD2	1.84	0.43
2:B:194:PHE:HA	2:B:195:PRO:HD3	1.74	0.43
1:A:53:PHE:O	1:A:64:SER:HA	2.18	0.43
2:B:223:LEU:O	2:B:224:GLU:C	2.57	0.43
1:A:311:PHE:CD2	1:A:311:PHE:C	2.92	0.43
1:A:321:PHE:N	1:A:321:PHE:CD2	2.86	0.43
1:A:353:LYS:HD2	2:B:224:GLU:OE2	2.18	0.43
1:A:199:TYR:CE1	3:A:999:ACO:H32	2.51	0.43
2:B:42:PRO:HA	2:B:45:GLU:HB2	2.00	0.43
1:A:111:ILE:HG22	1:A:111:ILE:O	2.18	0.43
2:B:58:TRP:CE3	2:B:86:ILE:HD12	2.53	0.43
2:B:119:GLN:NE2	2:B:147:GLU:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:TRP:CD1	2:B:103:PHE:HB3	2.50	0.43
1:A:290:ALY:HH33	1:A:329:VAL:CG1	2.49	0.43
1:A:308:LEU:HD23	1:A:312:TRP:CD1	2.54	0.43
1:A:6:PHE:CD2	1:A:106:ILE:HD12	2.54	0.43
1:A:293:PHE:O	1:A:293:PHE:HD1	2.02	0.43
2:B:44:TYR:HB3	2:B:209:TYR:OH	2.18	0.42
2:B:184:ARG:HG3	2:B:184:ARG:NH1	2.17	0.42
1:A:308:LEU:HD23	1:A:312:TRP:NE1	2.34	0.42
2:B:16:LEU:HA	2:B:16:LEU:HD12	1.81	0.42
2:B:173:ARG:NH1	2:B:173:ARG:HG3	2.35	0.42
1:A:212:ILE:N	1:A:212:ILE:CD1	2.83	0.42
2:B:167:GLU:O	2:B:167:GLU:HG3	2.20	0.42
1:A:241:LYS:HA	1:A:265:GLN:O	2.19	0.42
1:A:316:GLN:CD	1:A:316:GLN:O	2.58	0.42
1:A:19:TYR:CE2	1:A:396:GLN:HB2	2.55	0.42
2:B:64:GLN:O	2:B:64:GLN:HG3	2.18	0.42
1:A:83:ILE:O	1:A:189:ILE:HA	2.20	0.42
2:B:18:LEU:O	2:B:21:CYS:HB2	2.20	0.42
1:A:57:HIS:O	1:A:58:GLN:HB2	2.19	0.42
2:B:119:GLN:HE22	2:B:147:GLU:HB2	1.84	0.42
2:B:169:LYS:O	2:B:173:ARG:HG2	2.20	0.42
1:A:173:GLN:OE1	1:A:173:GLN:HA	2.19	0.42
1:A:100:VAL:HG12	1:A:221:TRP:CZ2	2.55	0.42
2:B:27:ALA:O	2:B:31:GLU:HG3	2.20	0.42
1:A:23:GLN:HA	1:A:50:GLN:O	2.19	0.42
1:A:165:GLU:CA	1:A:173:GLN:HB2	2.49	0.41
1:A:290:ALY:HE2	1:A:290:ALY:HH31	1.68	0.41
1:A:99:SER:OG	1:A:102:ASP:OD2	2.33	0.41
2:B:110:HIS:HA	2:B:118:GLU:CG	2.51	0.41
2:B:143:PRO:HD3	2:B:186:THR:CG2	2.51	0.41
2:B:60:ILE:HD12	2:B:216:TYR:HE1	1.86	0.41
2:B:152:TYR:HD1	2:B:152:TYR:N	2.17	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.86	0.41
1:A:79:ALA:HB3	1:A:185:ILE:HG21	2.03	0.41
1:A:56:PHE:CE1	1:A:61:VAL:HB	2.56	0.41
1:A:108:LEU:O	1:A:109:GLU:C	2.59	0.41
1:A:197:SER:C	1:A:198:GLN:HG3	2.40	0.41
1:A:270:PHE:CZ	1:A:290:ALY:HH31	2.56	0.41
2:B:188:LEU:C	2:B:190:PRO:HD3	2.41	0.41
2:B:162:ASP:OD1	2:B:164:ARG:NH1	2.53	0.41
2:B:36:ARG:HB3	2:B:36:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:NH1	1:A:318:ARG:CG	2.81	0.41
1:A:37:LYS:HZ3	1:A:38:ASP:H	1.69	0.41
1:A:253:ARG:O	1:A:257:ARG:HG3	2.20	0.41
2:B:57:PHE:O	2:B:61:VAL:HG23	2.21	0.41
1:A:219:MET:SD	1:A:244:ILE:CD1	3.09	0.41
1:A:13:VAL:CA	1:A:400:GLY:O	2.55	0.40
1:A:174:ASP:O	1:A:175:LEU:C	2.58	0.40
2:B:99:ASP:OD2	2:B:127:ILE:HD12	2.21	0.40
1:A:101:ARG:HA	1:A:221:TRP:CZ2	2.56	0.40
2:B:144:VAL:HA	2:B:145:PRO:HD3	1.86	0.40
2:B:106:THR:HG23	2:B:122:THR:OG1	2.21	0.40
2:B:103:PHE:O	2:B:103:PHE:CD1	2.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	387/438 (88%)	328 (85%)	46 (12%)	13 (3%)	5	29
2	B	209/232 (90%)	178 (85%)	25 (12%)	6 (3%)	6	34
All	All	596/670 (89%)	506 (85%)	71 (12%)	19 (3%)	5	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	121	GLN
1	A	176	TYR
1	A	320	GLU
1	A	37	LYS
1	A	127	ILE

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Mol	Chain	Res	Type
1	A	135	PRO
1	A	272	SER
2	B	95	SER
2	B	96	GLU
2	B	212	CYS
1	A	271	THR
1	A	373	GLU
2	B	223	LEU
1	A	300	GLU
2	B	111	GLY
1	A	275	ASN
1	A	317	GLU
2	B	152	TYR

### 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	359/398 (90%)	323 (90%)	36 (10%)	9	36
2	B	190/207 (92%)	171 (90%)	19 (10%)	9	36
All	All	549/605 (91%)	494 (90%)	55 (10%)	9	36

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	10	VAL
1	A	14	SER
1	A	18	GLU
1	A	27	LEU
1	A	28	GLU
1	A	34	THR
1	A	37	LYS
1	A	86	SER
1	A	101	ARG

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Mol	Chain	Res	Type
1	A	122	LYS
1	A	128	ARG
1	A	153	ARG
1	A	164	LYS
1	A	173	GLN
1	A	176	TYR
1	A	192	PHE
1	A	197	SER
1	A	198	GLN
1	A	208	SER
1	A	228	ARG
1	A	251	ARG
1	A	263	LEU
1	A	273	LYS
1	A	275	ASN
1	A	293	PHE
1	A	303	LEU
1	A	318	ARG
1	A	319	GLN
1	A	325	VAL
1	A	326	THR
1	A	364	TYR
1	A	383	ILE
1	A	384	ARG
1	A	388	LEU
1	A	393	THR
2	B	16	LEU
2	B	20	LYS
2	B	37	LEU
2	B	45	GLU
2	B	66	VAL
2	B	73	ARG
2	B	80	ILE
2	B	95	SER
2	B	110	HIS
2	B	113	GLU
2	B	117	LYS
2	B	129	LYS
2	B	151	SER
2	B	159	LEU
2	B	164	ARG
2	B	176	MET

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Mol	Chain	Res	Type
2	B	179	ILE
2	B	220	GLN
2	B	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	ALY	A	290	1	10,11,12	0.59	0	10,12,14	0.97	1 (10%)

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	ALY	A	290	1	-	2/8/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ALY	O-C-CA	-2.15	119.88	125.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	290	ALY	CH3-CH-NZ-CE
1	A	290	ALY	OH-CH-NZ-CE

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	290	ALY	8	0

## 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	$\# Z  > 2$
4	EDO	A	437	-	3,3,3	0.44	0	2,2,2	0.73	0
3	ACO	A	999	-	43,53,53	0.95	2 (4%)	55,79,79	2.21	17 (30%)

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	EDO	A	437	-	-	0/1/1/1	0/0/0/0
3	ACO	A	999	-	-	0/47/67/67	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ACO	C8A-N7A	2.24	1.38	1.34
3	A	999	ACO	C5A-C4A	3.08	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ACO	N3A-C2A-N1A	-8.81	122.15	128.89
3	A	999	ACO	C1B-N9A-C4A	-5.89	118.06	126.94
3	A	999	ACO	C4A-C5A-N7A	-3.94	105.85	109.48
3	A	999	ACO	C2P-C3P-N4P	-3.86	104.64	112.36
3	A	999	ACO	C7P-C6P-C5P	-3.65	106.30	112.31
3	A	999	ACO	O3A-P1A-O5B	-3.07	94.80	102.94
3	A	999	ACO	P2A-O3A-P1A	-2.46	125.81	132.73
3	A	999	ACO	O2B-C2B-C3B	-2.41	104.20	111.16
3	A	999	ACO	C7P-N8P-C9P	-2.36	117.86	122.53
3	A	999	ACO	O3A-P2A-O6A	2.09	108.48	102.94
3	A	999	ACO	CEP-CBP-CCP	2.10	111.23	108.50
3	A	999	ACO	CDP-CBP-CAP	2.22	113.40	109.34
3	A	999	ACO	O9A-P3B-O8A	2.24	115.93	107.38
3	A	999	ACO	C2A-N1A-C6A	2.58	123.37	118.77
3	A	999	ACO	C2B-C1B-N9A	2.88	118.69	114.29
3	A	999	ACO	CAP-C9P-N8P	2.89	122.88	116.47
3	A	999	ACO	C2P-S1P-C	3.61	124.14	101.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	437	EDO	2	0
3	A	999	ACO	3	0

## 5.7 Other polymers

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	393/438 (89%)	-0.12	2 (0%) 91 90	51, 85, 131, 149	0
2	B	213/232 (91%)	0.02	1 (0%) 91 90	66, 89, 130, 170	0
All	All	606/670 (90%)	-0.07	3 (0%) 91 90	51, 87, 131, 170	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	PRO	3.5
1	A	274	GLU	2.9
2	B	223	LEU	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	ALY	A	290	12/13	0.97	0.32	-	63,71,76,77	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	437	4/4	0.85	0.24	0.55	61,64,66,69	0
3	ACO	A	999	51/51	0.94	0.20	0.02	39,69,118,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.