



# Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2019 – 10:14 PM EDT

PDB ID : 1E8C  
Title : Structure of MurE the UDP-N-acetylmuramyl tripeptide synthetase from E. coli  
Authors : Gordon, E.J.; Chantala, L.; Dideberg, O.  
Deposited on : 2000-09-19  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

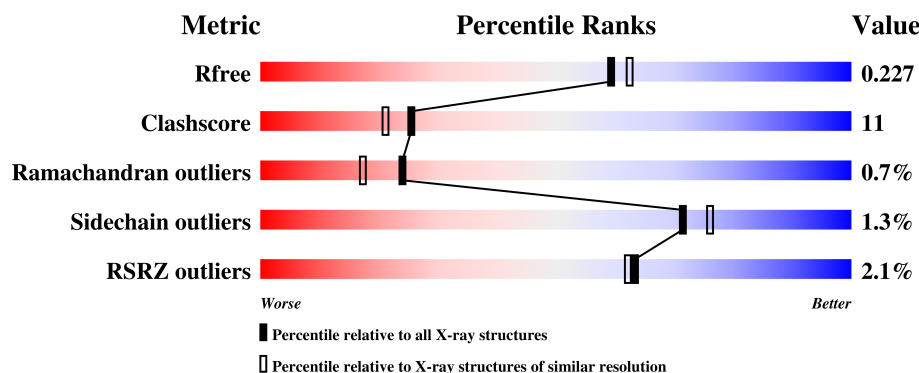
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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	498	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	498	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>19%</div> </div> </div>

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	CL	A	1001	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8093 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 UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMATE-2,6-DIAMINOPIMELATE LIGASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	16	5	1
			3772	2355	682	715	8	12			
1	B	497	Total	C	N	O	S	Se	24	5	0
			3787	2363	684	720	8	12			

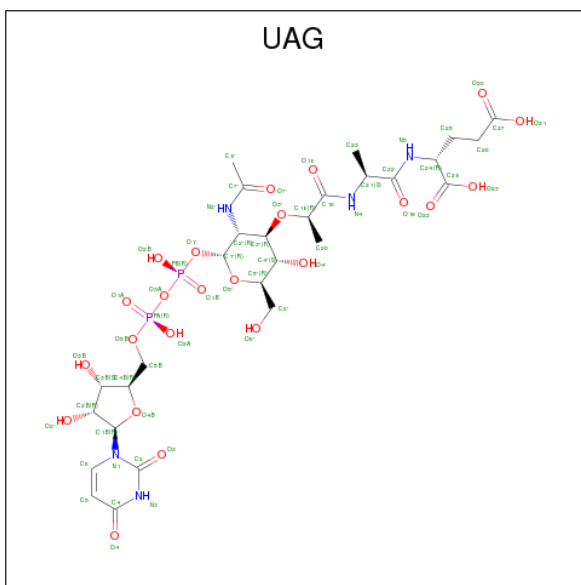
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	-	expression tag	UNP P22188
A	496	SER	-	expression tag	UNP P22188
A	497	HIS	-	expression tag	UNP P22188
A	498	HIS	-	expression tag	UNP P22188
B	495	ARG	-	expression tag	UNP P22188
B	496	SER	-	expression tag	UNP P22188
B	497	HIS	-	expression tag	UNP P22188
B	498	HIS	-	expression tag	UNP P22188

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

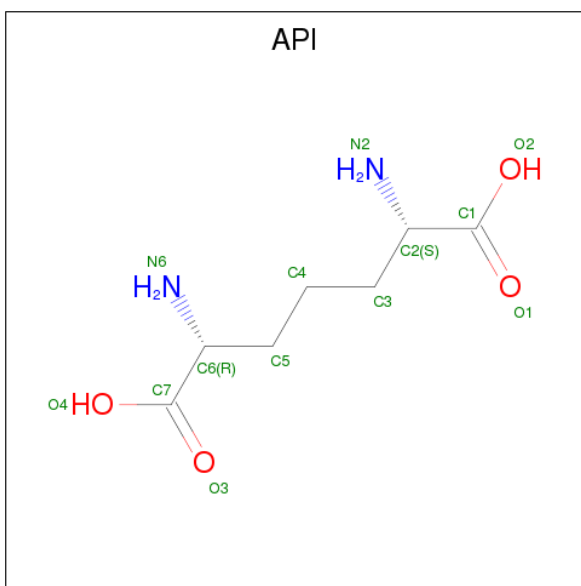
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE-D-GLUTAMATE (three-letter code: UAG) (formula: C<sub>28</sub>H<sub>43</sub>N<sub>5</sub>O<sub>23</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 57	C 28	N 5	O 22	P 2	0	0
3	B	1	Total 57	C 28	N 5	O 22	P 2	0	0

- Molecule 4 is 2,6-DIAMINOPIMELIC ACID (three-letter code: API) (formula:  $C_7H_{14}N_2O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 13	C 7	N 2	O 4	0	0
4	B	1	Total 13	C 7	N 2	O 4	0	0

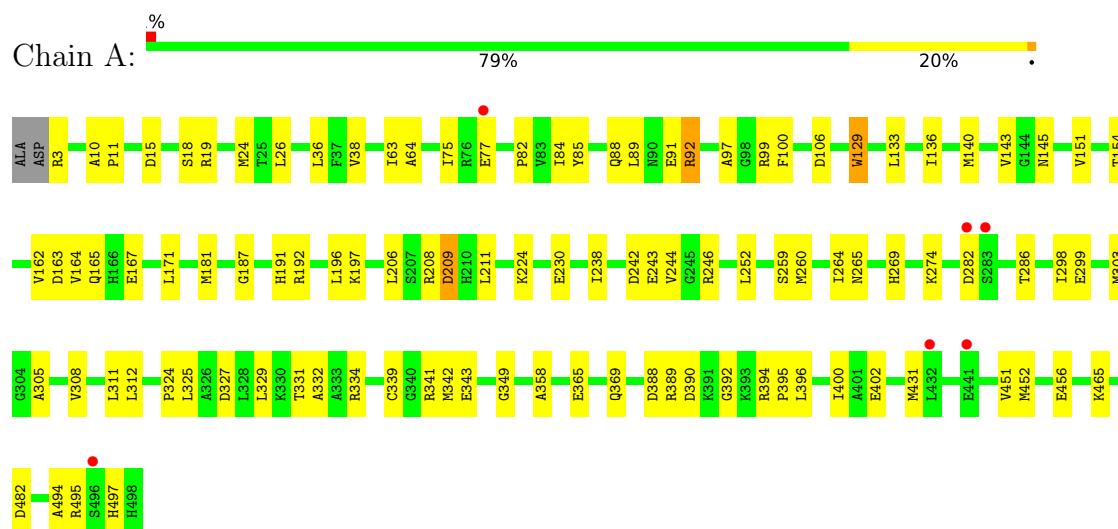
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0
5	B	187	Total 187	O 187	0	0

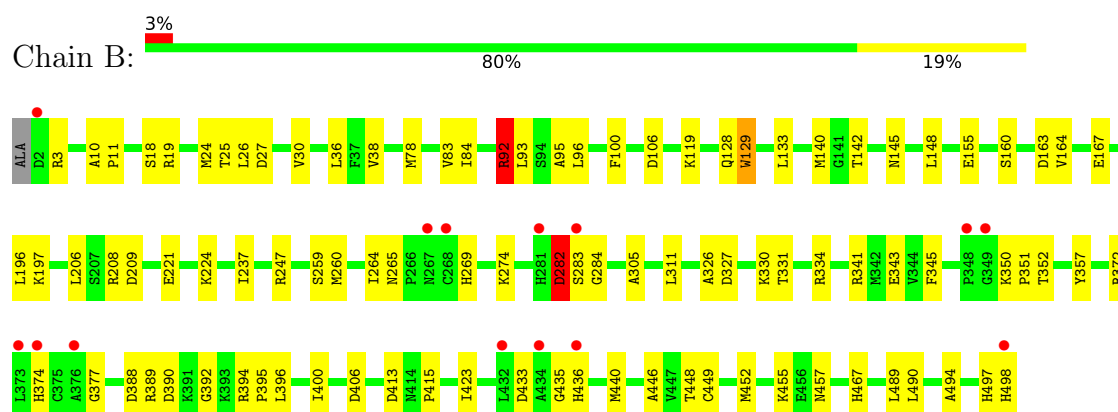
### 3 Residue-property plots

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

- Molecule 1: UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMATE--2,6-DIAMINOPIME LATE LIGASE



- Molecule 1: UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMATE--2,6-DIAMINOPIME LATE LIGASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.47Å 99.69Å 236.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.00 46.73 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.73-2.00) 98.1 (46.73-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.202 , 0.230 0.198 , 0.227	Depositor DCC
$R_{free}$ test set	7348 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, 0.333 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: API, KCX, UAG, CL

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	0.33	0/3846	0.62	1/5205 (0.0%)
1	B	0.33	0/3863	0.61	1/5227 (0.0%)
All	All	0.33	0/7709	0.61	2/10432 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ARG	O-C-N	5.35	131.25	122.70
1	A	136	ILE	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3772	0	3711	96	0
1	B	3787	0	3721	76	0
2	A	1	0	0	0	0
3	A	57	0	39	0	0
3	B	57	0	39	0	0
4	A	13	0	11	1	0
4	B	13	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	206	0	0	8	0
5	B	187	0	0	3	0
All	All	8093	0	7531	172	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 11.

All (172) 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:145:ASN:HB3	1:B:167[B]:GLU:OE2	1.24	1.31
1:A:145:ASN:HB3	1:A:167[B]:GLU:OE2	1.18	1.29
1:A:140:MSE:HE3	1:A:167[B]:GLU:OE1	1.22	1.27
1:A:140:MSE:HE3	1:A:167[B]:GLU:CD	1.53	1.26
1:B:140:MSE:HE3	1:B:167[B]:GLU:OE1	1.47	1.15
1:A:145:ASN:CB	1:A:167[B]:GLU:OE2	2.03	1.06
1:A:402:GLU:HB2	1:A:431:MSE:HE2	1.39	1.02
1:B:78[A]:MSE:HE3	1:B:83:VAL:HG21	1.45	0.99
1:B:25[B]:THR:HG22	1:B:27:ASP:H	1.30	0.97
1:A:260:MSE:HE1	1:A:305:ALA:HB1	1.47	0.92
1:B:145:ASN:CB	1:B:167[B]:GLU:OE2	2.18	0.88
1:B:260:MSE:HE1	1:B:305:ALA:HB1	1.56	0.86
1:A:389:ARG:HH11	1:A:389:ARG:HG3	1.41	0.86
1:B:389:ARG:HH11	1:B:389:ARG:HG3	1.39	0.85
1:A:77:GLU:OE1	1:A:82:PRO:HA	1.76	0.85
1:B:25[B]:THR:HG21	1:B:30:VAL:HG23	1.57	0.85
1:B:440:MSE:HE3	1:B:446:ALA:HA	1.60	0.83
1:A:208:ARG:NE	1:A:211:LEU:HD12	1.93	0.82
1:A:143:VAL:HG22	5:A:2078:HOH:O	1.83	0.79
1:A:75:ILE:HG12	1:A:84:ILE:HD12	1.65	0.77
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.49	0.77
1:B:265:ASN:H	1:B:269:HIS:HD2	1.34	0.76
1:B:106:ASP:OD1	1:B:197:LYS:HD2	1.86	0.76
1:B:265:ASN:H	1:B:269:HIS:CD2	2.05	0.75
1:A:331:THR:HG22	1:A:334:ARG:HH21	1.49	0.75
1:B:19:ARG:HG3	1:B:19:ARG:HH11	1.52	0.75
1:B:38:VAL:HG11	1:B:93:LEU:HD21	1.69	0.73
1:B:341:ARG:NH2	1:B:357:TYR:CD2	2.56	0.73
1:B:18:SER:O	1:B:19:ARG:HG3	1.89	0.72
1:A:298:ILE:HD11	1:A:329:LEU:HD23	1.71	0.72
1:B:341:ARG:HG3	1:B:341:ARG:HH11	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:CG2	5:A:2078:HOH:O	2.40	0.67
1:B:326:ALA:O	1:B:330:LYS:HG3	1.95	0.67
1:A:395:PRO:HG3	5:A:2182:HOH:O	1.96	0.65
1:A:140:MSE:SE	1:A:181:MSE:HE2	2.47	0.64
1:A:19:ARG:HD2	1:A:82:PRO:HG2	1.78	0.64
1:A:77:GLU:CD	5:A:2046:HOH:O	2.35	0.64
1:A:259:SER:HB3	1:A:264:ILE:HG12	1.80	0.63
1:A:208:ARG:NE	1:A:211:LEU:CD1	2.62	0.63
1:A:208:ARG:HE	1:A:211:LEU:HD12	1.62	0.62
1:B:394:ARG:HB2	1:B:395:PRO:HD3	1.80	0.62
1:A:365:GLU:O	1:A:369:GLN:HG3	1.98	0.62
1:A:389:ARG:HG3	1:A:389:ARG:NH1	2.14	0.62
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.65	0.62
1:B:264:ILE:HG13	1:B:274:LYS:HB3	1.80	0.62
1:B:25[B]:THR:HG21	1:B:30:VAL:CG2	2.29	0.61
1:B:395:PRO:HG3	5:B:2163:HOH:O	1.99	0.61
1:B:394:ARG:NH1	1:B:423:ILE:HG23	2.15	0.61
1:A:206:LEU:HD13	1:A:224:KCX:HD3	1.83	0.61
1:A:343:GLU:HA	1:A:497:HIS:CE1	2.35	0.61
1:A:365:GLU:HG3	1:A:400:ILE:HD12	1.82	0.60
1:A:77:GLU:OE1	1:A:82:PRO:CA	2.48	0.60
1:B:119:LYS:HG3	5:B:2071:HOH:O	2.03	0.59
1:A:163:ASP:O	1:A:167[A]:GLU:HG3	2.01	0.59
1:A:394:ARG:HB2	1:A:395:PRO:HD3	1.84	0.58
1:B:10:ALA:HB3	1:B:11:PRO:HD3	1.83	0.58
1:A:238:ILE:HD11	1:A:252:LEU:HD12	1.85	0.58
1:A:242:ASP:OD2	1:A:244:VAL:HB	2.04	0.58
1:A:77:GLU:OE2	5:A:2046:HOH:O	2.17	0.57
1:B:389:ARG:NH1	1:B:389:ARG:HG3	2.14	0.57
1:A:341:ARG:HG3	1:A:341:ARG:NH1	2.20	0.57
1:B:374:HIS:CG	1:B:374:HIS:O	2.58	0.57
1:B:343:GLU:HG2	1:B:494:ALA:CB	2.35	0.56
1:B:24:MSE:HE1	1:B:96:LEU:HG	1.88	0.56
1:B:206:LEU:HD13	1:B:224:KCX:HD3	1.88	0.55
1:B:259:SER:HB3	1:B:264:ILE:HG12	1.89	0.55
1:B:140:MSE:HE3	1:B:167[B]:GLU:CD	2.26	0.55
1:B:19:ARG:HG3	1:B:19:ARG:NH1	2.21	0.54
1:B:145:ASN:ND2	1:B:167[B]:GLU:OE1	2.41	0.54
1:A:140:MSE:CE	1:A:167[B]:GLU:CD	2.50	0.53
1:A:365:GLU:CG	1:A:400:ILE:HD12	2.38	0.53
1:A:388:ASP:O	1:A:389:ARG:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:THR:HG22	1:A:334:ARG:NH2	2.19	0.53
1:B:350:LYS:HE2	1:B:489:LEU:O	2.09	0.53
1:B:3:ARG:HD3	1:B:100:PHE:O	2.08	0.52
1:A:298:ILE:HD11	1:A:329:LEU:CD2	2.38	0.52
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.73	0.52
1:A:264:ILE:HB	1:A:274:LYS:HD3	1.90	0.52
1:A:208:ARG:O	1:A:209:ASP:HB2	2.09	0.52
1:A:24:MSE:HE2	1:A:162:VAL:HG22	1.92	0.52
1:B:331:THR:HG22	1:B:334:ARG:HH21	1.75	0.52
1:A:264:ILE:HG13	1:A:274:LYS:HB3	1.92	0.51
1:A:392:GLY:O	1:A:395:PRO:HD2	2.10	0.51
1:B:396:LEU:O	1:B:400:ILE:HG12	2.10	0.51
1:A:88[A]:GLN:OE1	1:A:91:GLU:OE2	2.29	0.51
1:B:351:PRO:HB3	1:B:455:LYS:O	2.10	0.51
1:A:26:LEU:HD23	1:A:38:VAL:HB	1.93	0.51
1:A:343:GLU:HG2	1:A:494:ALA:HB2	1.94	0.50
1:A:89:LEU:HA	1:A:92:ARG:HG3	1.92	0.50
1:B:389:ARG:CG	1:B:389:ARG:NH1	2.74	0.50
1:B:392:GLY:O	1:B:395:PRO:HD2	2.12	0.50
1:A:265:ASN:H	1:A:269:HIS:CE1	2.29	0.49
1:A:75:ILE:HG12	1:A:84:ILE:CD1	2.39	0.49
1:A:208:ARG:HE	1:A:211:LEU:CD1	2.24	0.49
1:A:396:LEU:O	1:A:400:ILE:HG12	2.12	0.49
1:A:3:ARG:NH1	1:A:3:ARG:HG3	2.26	0.49
1:A:465:LYS:HB2	1:A:482:ASP:OD2	2.12	0.49
1:B:84:ILE:HD12	1:B:84:ILE:N	2.27	0.49
1:A:343:GLU:HG2	1:A:494:ALA:CB	2.44	0.48
1:A:3:ARG:CD	1:A:100:PHE:HA	2.43	0.48
1:B:92:ARG:O	1:B:95:ALA:HB3	2.14	0.48
1:B:341:ARG:CG	1:B:341:ARG:HH11	2.22	0.48
1:B:350:LYS:HD3	1:B:490:LEU:CD2	2.44	0.48
1:A:324:PRO:HG2	1:A:327:ASP:HB2	1.96	0.47
1:B:311:LEU:HD23	1:B:311:LEU:C	2.34	0.47
1:B:24:MSE:HE3	1:B:36:LEU:CD2	2.44	0.47
1:A:308:VAL:O	1:A:312:LEU:HG	2.15	0.47
1:B:237:ILE:N	1:B:237:ILE:HD12	2.29	0.47
1:B:436:HIS:ND1	1:B:436:HIS:O	2.44	0.47
1:B:388:ASP:O	1:B:389:ARG:HG3	2.15	0.46
1:A:97:ALA:HB3	1:A:165:GLN:HG3	1.98	0.46
1:A:91:GLU:HG3	5:A:2056:HOH:O	2.16	0.46
1:A:24:MSE:HE3	1:A:38:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:O	1:A:19:ARG:HG3	2.16	0.46
1:B:282:ASP:C	1:B:284:GLY:N	2.69	0.46
1:A:389:ARG:HE	4:A:1499:API:C1	2.29	0.45
1:A:106:ASP:OD1	1:A:197:LYS:HD2	2.17	0.45
1:A:303:MSE:HE2	1:A:342:MSE:CE	2.46	0.45
1:B:413:ASP:O	1:B:415[B]:PRO:HD3	2.17	0.45
1:A:298:ILE:HD12	1:A:332:ALA:CB	2.46	0.45
1:A:99:ARG:HB3	1:A:99:ARG:HH11	1.81	0.45
1:B:142:THR:HG22	1:B:467:HIS:CE1	2.51	0.45
1:A:495:ARG:HB2	5:A:2204:HOH:O	2.15	0.45
1:B:221:GLU:CD	1:B:247:ARG:HH22	2.19	0.45
1:B:497:HIS:O	1:B:498:HIS:OXT	2.35	0.45
1:B:128:GLN:HA	1:B:148:LEU:HD11	1.98	0.45
1:B:208:ARG:O	1:B:209:ASP:HB2	2.16	0.45
1:A:451:VAL:HG12	1:A:452:MSE:HE2	2.00	0.44
1:B:352:THR:HG21	1:B:374:HIS:NE2	2.32	0.44
1:A:208:ARG:HG3	1:A:209:ASP:N	2.32	0.44
1:A:151:VAL:HG22	5:A:2082:HOH:O	2.17	0.44
1:B:282:ASP:O	1:B:284:GLY:N	2.50	0.44
1:A:389:ARG:NH1	1:A:389:ARG:CG	2.77	0.44
1:A:343:GLU:HG3	1:A:497:HIS:CE1	2.53	0.43
1:A:3:ARG:HD3	1:A:100:PHE:HA	2.00	0.43
1:A:286:THR:HG23	1:A:299:GLU:OE2	2.18	0.43
1:A:10:ALA:HB3	1:A:11:PRO:HD3	1.99	0.43
1:A:19:ARG:NH1	1:A:19:ARG:HG3	2.32	0.43
1:A:64:ALA:O	1:A:85:TYR:HA	2.19	0.43
1:A:311:LEU:HD23	1:A:311:LEU:C	2.38	0.43
1:A:187:GLY:HA2	1:A:192:ARG:HD2	2.00	0.43
1:A:36:LEU:HD11	1:A:63:ILE:HG13	2.00	0.42
1:B:26:LEU:HD23	1:B:38:VAL:HB	2.00	0.42
1:A:243:GLU:HG2	1:A:246:ARG:NH1	2.34	0.42
1:B:264:ILE:CG1	1:B:274:LYS:HB3	2.48	0.42
1:A:349:GLY:HA2	1:A:456:GLU:OE1	2.19	0.42
1:B:160:SER:O	1:B:164:VAL:HG23	2.20	0.42
1:A:325:LEU:O	1:A:329:LEU:HG	2.20	0.42
1:B:341:ARG:NH2	1:B:357:TYR:CE2	2.88	0.42
1:B:129:TRP:O	1:B:133:LEU:HD23	2.20	0.41
1:B:433:ASP:C	1:B:435:GLY:H	2.23	0.41
1:B:164:VAL:HG11	1:B:196:LEU:HD11	2.01	0.41
1:B:440:MSE:HE1	1:B:449:CYS:CB	2.51	0.41
1:B:377:GLY:HA3	1:B:457:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:THR:HA	1:A:334:ARG:NH2	2.35	0.41
1:B:345:PHE:HB3	1:B:490:LEU:HD12	2.01	0.41
1:A:15:ASP:OD2	1:A:75:ILE:HD12	2.21	0.41
1:A:91:GLU:HG2	1:A:191:HIS:CE1	2.56	0.41
1:B:341:ARG:CG	1:B:341:ARG:NH1	2.80	0.41
1:A:145:ASN:ND2	1:A:154:THR:HG21	2.36	0.41
1:B:448:THR:O	1:B:452:MSE:HG2	2.21	0.41
1:A:129:TRP:O	1:A:133:LEU:HD23	2.21	0.41
1:A:164:VAL:HG11	1:A:196:LEU:HD11	2.03	0.41
1:A:208:ARG:CZ	1:A:211:LEU:HD12	2.48	0.41
1:B:394:ARG:NH1	5:B:2158:HOH:O	2.53	0.41
1:B:24:MSE:HE3	1:B:36:LEU:HD21	2.03	0.40
1:B:343:GLU:HG2	1:B:494:ALA:HB2	2.03	0.40
1:B:440:MSE:HE1	1:B:449:CYS:HB2	2.04	0.40
1:B:372:ARG:HH22	1:B:406:ASP:CG	2.24	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/498 (100%)	480 (96%)	14 (3%)	4 (1%)	21	14
1	B	499/498 (100%)	483 (97%)	13 (3%)	3 (1%)	27	21
All	All	997/996 (100%)	963 (97%)	27 (3%)	7 (1%)	24	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASP
1	B	282	ASP
1	B	283	SER

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Mol	Chain	Res	Type
1	B	390	ASP
1	A	390	ASP
1	A	209	ASP
1	A	358	ALA

### 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	391/376 (104%)	387 (99%)	4 (1%)	78	83
1	B	393/376 (104%)	387 (98%)	6 (2%)	67	72
All	All	784/752 (104%)	774 (99%)	10 (1%)	71	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	129	TRP
1	A	230	GLU
1	A	339	CYS
1	B	92	ARG
1	B	129	TRP
1	B	155	GLU
1	B	163	ASP
1	B	282	ASP
1	B	327	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	90	ASN
1	A	117	ASN
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	156	ASN
1	A	186	HIS
1	A	263	HIS
1	A	336	GLN
1	B	44	GLN
1	B	90	ASN
1	B	124	GLN
1	B	156	ASN
1	B	166	HIS
1	B	219	HIS
1	B	269	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	KCX	A	224	1	8,11,12	1.26	2 (25%)	5,12,14	2.15	1 (20%)
1	KCX	B	224	1	8,11,12	1.12	1 (12%)	5,12,14	2.72	1 (20%)

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	KCX	A	224	1	-	0/6/10/12	0/0/0/0
1	KCX	B	224	1	-	0/6/10/12	0/0/0/0



All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	KCX	CA-C	2.25	1.53	1.50
1	B	224	KCX	CE-NZ	2.38	1.50	1.45
1	A	224	KCX	CE-NZ	2.54	1.51	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	KCX	CE-NZ-CX	-5.70	116.00	123.28
1	A	224	KCX	CE-NZ-CX	-4.42	117.63	123.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	224	KCX	1	0
1	B	224	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
3	UAG	A	1498	4	48,59,60	2.28	13 (27%)	62,86,88	2.14	19 (30%)
4	API	A	1499	3	4,12,12	1.52	2 (50%)	3,15,15	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UAG	B	1498	4	48,59,60	2.28	13 (27%)	62,86,88	2.18	19 (30%)
4	API	B	1499	3	4,12,12	1.22	1 (25%)	3,15,15	1.03	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
3	UAG	A	1498	4	-	0/45/91/92	0/3/3/3
4	API	A	1499	3	-	0/6/14/14	0/0/0/0
3	UAG	B	1498	4	-	0/45/91/92	0/3/3/3
4	API	B	1499	3	-	0/6/14/14	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1498	UAG	C21-N4	-6.31	1.33	1.45
3	B	1498	UAG	C21-N4	-6.16	1.33	1.45
3	B	1498	UAG	O2'-C2B	-2.51	1.37	1.43
3	A	1498	UAG	O2'-C2B	-2.35	1.37	1.43
3	B	1498	UAG	C3B-C4B	-2.21	1.47	1.53
3	A	1498	UAG	C3B-C4B	-2.19	1.47	1.53
4	B	1499	API	C6-N6	2.03	1.51	1.47
3	A	1498	UAG	C22-N5	2.09	1.38	1.34
4	A	1499	API	C2-N2	2.12	1.52	1.47
4	A	1499	API	C6-N6	2.16	1.52	1.47
3	B	1498	UAG	C22-N5	2.19	1.38	1.34
3	B	1498	UAG	C2-N3	2.24	1.42	1.38
3	A	1498	UAG	C2-N3	2.36	1.42	1.38
3	A	1498	UAG	PB-O1'	2.54	1.67	1.60
3	A	1498	UAG	PA-O5B	2.58	1.69	1.59
3	B	1498	UAG	PB-O1'	2.76	1.67	1.60
3	A	1498	UAG	C4'-C5'	2.84	1.59	1.53
3	B	1498	UAG	C4'-C5'	2.84	1.59	1.53
3	B	1498	UAG	C19-N4	2.85	1.40	1.34
3	B	1498	UAG	PA-O5B	2.86	1.70	1.59
3	A	1498	UAG	C19-N4	2.97	1.40	1.34
3	A	1498	UAG	C3'-C2'	3.43	1.58	1.53
3	B	1498	UAG	C1'-C2'	3.69	1.59	1.53
3	B	1498	UAG	C3'-C2'	3.83	1.59	1.53
3	A	1498	UAG	C1'-C2'	4.29	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1498	UAG	C6-N1	5.88	1.43	1.35
3	B	1498	UAG	C6-N1	6.27	1.43	1.35
3	B	1498	UAG	C4-N3	7.01	1.45	1.33
3	A	1498	UAG	C4-N3	7.15	1.45	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1498	UAG	C25-C24-C28	-4.13	106.23	112.18
3	A	1498	UAG	O5'-C1'-O1'	-4.02	106.11	111.36
3	A	1498	UAG	C25-C24-C28	-4.01	106.41	112.18
3	B	1498	UAG	O5'-C1'-O1'	-3.87	106.30	111.36
3	B	1498	UAG	C1'-C2'-N2'	-2.64	106.33	110.96
3	A	1498	UAG	C22-C21-N4	-2.55	105.28	111.61
3	A	1498	UAG	C5B-C4B-C3B	-2.40	106.16	115.21
3	A	1498	UAG	C5-C4-N3	-2.30	118.12	123.28
3	A	1498	UAG	O3'-C18-C19	-2.26	106.29	111.17
3	B	1498	UAG	C5-C4-N3	-2.26	118.22	123.28
3	B	1498	UAG	C22-C21-N4	-2.23	106.09	111.61
3	B	1498	UAG	C5B-C4B-C3B	-2.21	106.90	115.21
3	B	1498	UAG	O3'-C18-C19	-2.18	106.46	111.17
3	A	1498	UAG	C1'-C2'-N2'	-2.16	107.17	110.96
3	B	1498	UAG	C23-C21-C22	-2.14	106.04	110.14
3	A	1498	UAG	C23-C21-C22	-2.04	106.23	110.14
3	B	1498	UAG	O4B-C4B-C3B	2.04	109.16	105.14
3	A	1498	UAG	O4B-C4B-C3B	2.15	109.38	105.14
3	B	1498	UAG	C25-C24-N5	2.20	113.41	110.19
3	A	1498	UAG	C25-C24-N5	2.37	113.67	110.19
3	B	1498	UAG	C21-N4-C19	2.38	126.47	121.28
3	B	1498	UAG	O2A-PA-O1A	2.39	124.21	112.21
3	A	1498	UAG	O2A-PA-O1A	2.40	124.26	112.21
3	A	1498	UAG	O2'-C2B-C3B	2.67	120.47	111.80
3	A	1498	UAG	O4B-C4B-C5B	2.68	118.26	109.38
3	A	1498	UAG	C21-N4-C19	2.72	127.19	121.28
3	B	1498	UAG	O2'-C2B-C3B	2.73	120.67	111.80
3	A	1498	UAG	C23-C21-N4	2.87	115.67	110.36
3	B	1498	UAG	C23-C21-N4	3.11	116.13	110.36
3	B	1498	UAG	O4B-C4B-C5B	3.12	119.73	109.38
3	A	1498	UAG	O5B-C5B-C4B	3.20	120.03	108.99
3	B	1498	UAG	O5B-C5B-C4B	3.62	121.46	108.99
3	B	1498	UAG	C2B-C3B-C4B	3.93	110.12	102.60
3	A	1498	UAG	C2B-C3B-C4B	3.94	110.14	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1498	UAG	O4B-C1B-N1	7.12	121.97	108.06
3	B	1498	UAG	O4B-C1B-N1	7.46	122.63	108.06
3	A	1498	UAG	PB-O3A-PA	7.80	157.36	132.57
3	B	1498	UAG	PB-O3A-PA	8.01	158.02	132.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1499	API	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, 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	483/498 (96%)	-0.02	6 (1%) 79 78	17, 32, 49, 62	11 (2%)
1	B	484/498 (97%)	0.02	14 (2%) 51 51	18, 33, 52, 65	16 (3%)
All	All	967/996 (97%)	0.00	20 (2%) 63 62	17, 32, 51, 65	27 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	6.5
1	B	374	HIS	5.2
1	B	283	SER	3.5
1	A	432	LEU	3.0
1	B	498	HIS	2.9
1	A	282	ASP	2.9
1	A	496	SER	2.9
1	B	432	LEU	2.8
1	B	436	HIS	2.8
1	B	434	ALA	2.6
1	B	267	ASN	2.3
1	A	77	GLU	2.2
1	B	349	GLY	2.2
1	B	268	CYS	2.2
1	B	376	ALA	2.2
1	B	2	ASP	2.1
1	B	373	LEU	2.1
1	B	348	PRO	2.0
1	B	281	HIS	2.0
1	A	441	GLU	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	B	224	12/13	0.96	0.12	17,20,25,27	0
1	KCX	A	224	12/13	0.98	0.11	19,21,28,28	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	1001	1/1	0.60	0.73	34,34,34,34	0
4	API	B	1499	13/13	0.62	0.28	52,63,69,75	0
4	API	A	1499	13/13	0.70	0.30	60,66,74,75	0
3	UAG	B	1498	57/58	0.96	0.13	22,32,45,52	0
3	UAG	A	1498	57/58	0.96	0.12	21,30,46,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.